



# **ReaxFF Manual**

*Release 2017*

**[www.scm.com](http://www.scm.com)**

**Apr 12, 2018**



# CONTENTS

<b>1</b>	<b>General</b>	<b>1</b>
1.1	Release 2017 . . . . .	1
<b>2</b>	<b>Ensembles</b>	<b>3</b>
2.1	Nose-Hoover chains NVT ensemble . . . . .	3
2.2	AH and PRH NPT ensemble with NHC . . . . .	3
<b>3</b>	<b>eReaxff: classical treatment of the explicit electron</b>	<b>5</b>
<b>4</b>	<b>FF Optimizer: framework for force field parameter optimizers</b>	<b>7</b>
4.1	Input files . . . . .	7
4.2	Control parameters . . . . .	7
<b>5</b>	<b>MCFF Optimizer: Monte Carlo force field parameter optimizer</b>	<b>9</b>
5.1	Input files . . . . .	9
5.2	Control parameters . . . . .	9
5.3	Results . . . . .	10
5.4	Run-time control . . . . .	11
<b>6</b>	<b>Grand Canonical Monte Carlo (GCMC)</b>	<b>13</b>
6.1	General info . . . . .	13
6.2	Input . . . . .	14
6.3	Output . . . . .	17
6.4	Code Details . . . . .	18
6.5	Tutorial: Discharge voltages . . . . .	19
<b>7</b>	<b>force-bias Monte Carlo (fbMC)</b>	<b>27</b>
<b>8</b>	<b>The Molecule Gun</b>	<b>29</b>
<b>9</b>	<b>TRAVIS: A Trajectory Analyzer and Visualizer</b>	<b>31</b>
<b>10</b>	<b>Other new features and fixes</b>	<b>33</b>
10.1	Molecular charges . . . . .	33
10.2	ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order . . . . .	33
10.3	Correction for torsion angles asymptotics . . . . .	33
10.4	LG dispersion . . . . .	34
10.5	ChemTraYzer . . . . .	34
10.5.1	General information . . . . .	34
10.5.2	Command line execution . . . . .	34
10.5.3	Results . . . . .	35

10.6 Repeating the unit cells . . . . .	35
<b>11 Troubleshooting</b>	<b>37</b>
11.1 Geometry optimization . . . . .	37
<b>12 Warnings</b>	<b>39</b>
<b>13 Included Forcefields</b>	<b>41</b>
<b>14 Included Forcefields (development)</b>	<b>53</b>
<b>15 Required Citations</b>	<b>65</b>
15.1 General References . . . . .	65
15.2 Feature References . . . . .	65
15.3 External programs and Libraries . . . . .	66

## 1.1 Release 2017

In comparison to ADF-ReaxFF 2016, the 2017 release offers the following new functionality:

- Nose-Hoover chains thermostat
- Anderson barostat with a Nose-Hoover chains thermostat (isotropic, anisotropic and full cell fluctuation)
- e-Reax - dynamics with explicit electrons
- Extendable FF Optimizer framework
- Vibrational frequency analysis
- Quasi-Newton geometry optimization
- Improved molecule gun



## ENSEMBLES

Currently the following ensembles are implemented in the ReaxFF program:

- NVE
- NVT with a Berendsen thermostat (see the pdf manual for details)
- NVT with a Nose-Hoover chain (NHC) thermostat
- NPT with a Berendsen baro- and thermostat (see the pdf manual for details)
- Anderson-Hoover (AH) or Parrinello-Rahman-Hoover (PRH) NPT with NHC thermostats

### 2.1 Nose-Hoover chains NVT ensemble

Both the NHC-NVT and the AH-NPT are implemented following the paper by G.J. Martyna et al. [G J Martyna, M E Tuckerman, D J Tobias, M L Klein, Mol. Phys. 87 (1996) 1117]. The following parameters are used: N\_c=5, N\_ys=5, Nchains=10. The NHC-NVT ensemble is invoked by setting imdmet=2 in the control file. The tdamp control parameter ( $\tau_t$ ) is used to determine the first thermostat mass as  $Q = N_{free}kT_{set}\tau_t^2$ . It should be noted that the  $\tau_t$  in the Nose-Hoover method corresponds to the period of the characteristic oscillations of the system, which is different from the  $\tau$  in the Berendsen thermostat where it determines the relaxation time. Relaxation of the system with a Nose-Hoover thermostat usually takes longer than with the Berendsen one with the same  $\tau$ .

The temperature regimes and zones specified via the tregime.in file can also be used with the NHC thermostat the same way as with the Berendsen one.

### 2.2 AH and PRH NPT ensemble with NHC

The Anderson-Hoover NPT ensemble is invoked by setting imdmet=9 in the control file. Everything written above about the NHC thermostat applies also to the thermostat part of the AH-NPT. The particle thermostat and the barostat are controlled by two different chains. The masses in the barostat thermostat chain are determined by the tdamp parameter as  $Q_p = kT_{set}\tau_t^2$ . The pdamp control parameter  $\tau_p$  defines the barostat mass as  $W = (N_{free} + 3)kT_{set}\tau_p^2$ . Similar to the NHC thermostat, the  $\tau_p$  here corresponds to the period of the characteristic pressure fluctuations of the system.

For an anisotropic NPT dynamics one should specify imdmet=10 (fixed cell angles) or imdmet=11 (full cell fluctuations). It should be noted that the anisotropic NPT dynamics has not been well tested yet and thus it should be considered experimental.





## EREAXFF: CLASSICAL TREATMENT OF THE EXPLICIT ELECTRON

The eReaxFF implementation in the SCM ReaxFF program is based on the paper [J. Chem.Theory Comput 12, 3463 (2016) (<http://dx.doi.org/10.1021/acs.jctc.6b00432>)] and on the prototype code obtained from the group of Adri van Duin. It was, however, largely rewritten by SCM to meet our coding standards and to maximize performance.

An eReaxFF calculation requires the following additional force-field parameters to be defined (equation numbers are referring to the eReaxFF paper):

- The header of the force-field file must begin with the “[ ereaxff acks2 ]” string,
- General parameter 27: the currently reserved  $p_{elho}$  parameter in the unpublished electron-hole interaction equation (which is still highly experimental and is subject to change),
- General parameter 37: the Gauss exponent parameter  $p_{val}$  describing the free electron, Eq(3),
- Atomic parameter 24: the  $\alpha$  parameter in Eq(2),
- Atomic parameter 27: the  $\beta$  parameter in Eq(2),
- Atomic parameter 13: the  $p_{ij}^{xel2}$  parameter in Eq(4d),
- Bond parameter 16: the  $p_{ij}^{xel1}$  parameter in Eq(4d).

Additionally, since the eReaxFF method is usually coupled to the ACKS2 charge equilibration method, the ACKS2-related parameters should also be defined.

In the input geometry file, the explicit electrons are called ‘El’ and the holes are ‘Ho’ (yes we are aware that the latter clashes with holmium but this is what the original authors are using).

It should be noted that the eReaxFF implementation is considered experimental so the users are advised to contact Adri van Duin regarding its use.



## FF OPTIMIZER: FRAMEWORK FOR FORCE FIELD PARAMETER OPTIMIZERS

The FF Optimizer is a base module that can be extended with other modules that implement specific optimization methods. The FFOptimizer module offers methods to compute an error function (also known as the cost function) and its first and second derivatives with respect to the force-field parameter values.

### 4.1 Input files

In order to calculate properties of the training set error function with respect to the force-field parameters, the files listed below must be present in the directory where the reaxff program is executed.

- *iopt* – file containing a line of text with a single number on it. If the number is 6 then the first partial derivatives of the error function with respect to force-field parameters will be computed by finite difference. This option requires  $2*N + 1$  error function evaluations, where N is the number of variable force-field parameters. If *iopt*=8, then both the first and the second derivatives will be calculated. The eigenvalues and eigenvectors of the obtained Hessian matrix will also be computed. In this case,  $N^2 + N + 1$  function evaluations will be done. Note: calculation of the derivatives can be very slow so make sure you run it on as many processors as possible. A rule of thumb is that the number of processor cores should be equal or larger than the number of variable parameters.
- *ffield* – the initial force-field file.
- *ffield\_bool* – contains 1.0 or 0.0 as a flag whether the corresponding value is to be variable or not (this file has the same format as *ffield*).
- *trainset.in* – file with test values, the same as in the original reaxff force-field optimization, see page 27 of the ReaxFF User Manual.
- *geo* – file with test geometries in the BGF format, the same as in the original reaxff force-field optimization. Geometries of different molecules in this file must be concatenated.
- *control* – in addition to general ReaxFF control parameters it also contains the FFOptimizer-related ones explained below.

### 4.2 Control parameters

The following control parameters are related to the FFOptimizer. The default value for each parameter is given in parentheses.

- *ffstp* – the delta used for calculating first and second derivatives by finite differences (0.01).

- *ffdedi* – If running in parallel and *ffdedi* is set to 1 then the master process will run as a dedicated dispatcher and will not perform any computations. The default value depends on the number of processors used in the calculation (1 for  $N_{\text{proc}} > 3$ ).

## MCFF OPTIMIZER: MONTE CARLO FORCE FIELD PARAMETER OPTIMIZER

The MCFF Optimizer uses a Monte Carlo approach to finding the best fit force field for the given training set. It is based on the paper by E. Iype et. al. (<http://dx.doi.org/10.1002/jcc.23246>) In the following sections, the input and output of the MCFF Optimizer are described.

A worked out example on building a training set and optimizing a ReaxFF force field with MCFF is on our [workshop pages](https://www.scm.com/adf-modeling-suite/adf-hands-on-workshops/advanced-2-day-reaxff-workshop/) (<https://www.scm.com/adf-modeling-suite/adf-hands-on-workshops/advanced-2-day-reaxff-workshop/>).

### 5.1 Input files

In addition to files specified in the FF Optimizer section the following files must be present in the directory where the reaxff program is executed.

- *iopt* – file containing a single text line with 4 on it. This will instruct reaxff to perform a Monte-Carlo force-field optimization.
- *ffield\_min* – minimum values for each force-field value (this file has the same format as *ffield*).
- *ffield\_max* – maximum values for each force-field value (this file has the same format as *ffield*).

The *mccfpt\_water* example in the *examples/reaxff* directory demonstrates the use of the MCFFOptimizer. Note however that this example is not physically meaningful. For example, many atomic force-field parameters are allowed to vary in a very broad range, which is the same for all elements. In practice, you will want to set the range for each element separately.

### 5.2 Control parameters

The following control parameters are related to MCFFOptimizer. The default value for each parameter is given in parentheses.

- *mccfit* - number of MC iterations (10000). Since the Monte-Carlo method does not have any notion of convergence the optimization is stopped after *mccfit* iterations.
- *mcbeta* - initial MC beta parameter in the acceptance probability calculation  $P = \exp(-\beta\Delta E)$  (1.0). Here,  $\Delta E$  is a difference in the error function between the current and the best step so far. If the current step is the best, it is always accepted. Otherwise, the acceptance probability is calculated using the formula above and it is calculated with a random number from the (0,1) range. The optimal value of beta depends on values of the error function.

- *mcdbet* - simulated annealing: increase the beta parameter by this value at each step (0.0). A positive *mcdbet* value means that the probability to take a step that increases the error function will decrease over time. This has the same effect as decreasing the temperature in the classical molecular Monte-Carlo method.
- *mcbzca* - simulated annealing: divide the beta parameter by this value at each step (1.0). A value of *mcbzca* less than 1.0 has an effect similar to positive *mcdbet*.
- *mcacpf* - probability to vary a variable at each step (0.2). To avoid taking very large steps only some of the variables are varied at each step (selected randomly).
- *mcrxdd* - number of steps to divide the parameter range between *ffield\_min* and *ffield\_max* into (100).
- *mcstep* - initial max step size in units of  $\text{range}/\text{mcrxdd}$ , where  $\text{range}$  = difference between *ffield\_max* and *ffield\_min* values (1.0).
- *mcmxst* - maximum allowed value of max step size (100);
- *mcscps* - factor to scale max step size to satisfy acceptance tolerance (1.1);
- *mctart* - target acceptance rate, percent (30.0);
- *mcmart* - max acceptance rate, percent (70.0);
- *mcmini* - if not 0, minimize the best force-field parameter set after so many iterations (0). The optimization is performed only if the best set has changed since the previous minimization. The minimization employed here is gradient-free and relatively slow so it should not be used too frequently.
- *replic* - number of replicas to try at each step (1). At each step, *replic* Monte-Carlo steps are done and the one with the lowest error is selected for the next iteration.

**Relation between *mcrxdd*, *mcstep*, *mcmxst*, and *mcscps*.** The allowed range for each parameter is divided into *mcrxdd* steps. At each optimization step, a number of force-field parameters is changed by a random value in the range  $(-\Delta x, \Delta x)$ , where  $\Delta x = \text{mcstep} * (X_{\text{max}} - X_{\text{min}}) / \text{mcrxdd}$ . Here,  $X_{\text{max}}$  and  $X_{\text{min}}$  are values of this parameter from *ffield\_max* and *ffield\_min*, respectively. When performing optimization, the program keeps track of the average acceptance rate and adjusts *mcstep* up or down by the *mcscps* factor to keep the acceptance rate close to *mctart*. If the acceptance rate is too low the step size is decreased to allow searching for a smaller parameter space. The *mcstep* value can never be larger than *mcmxst*.

It should be noted that the value of the MC step size (and thus all the parameters discussed in this section) applies to all force-field parameters to the same extent, which means that it is very important to select the min and max parameter values very carefully. The rule of thumb here is that the range should be as small as possible covering only the physically meaningful values.

## 5.3 Results

Main results of the MCFFOptimizer are saved in the following files:

- *ffield\_best* - force-field file corresponding to the lowest error value
- *ffield\_last* - the most recent accepted force-filed
- *MCFFOptimizer.log* - summary of iterations including the error function value, number of changed and bounded force-field parameters, cumulative number of accepted and rejected steps at each step. Also the current MC parameters such as the  $\beta$  value and the acceptance rate, are shown, as well as the elapsed time in seconds.
- *fort.99* - the error function breakdown for the latest step

## 5.4 Run-time control

The progress of the force-field optimization can be controlled by changing parameters in the *istop* file present in the calculation directory. The file is read every 10 iterations. The parameters are explained below:

- StopKey - replace 0 with 1 to stop the calculation
- Beta - the current  $\beta$  value corresponding to the *mcbeta* control parameter
- Command - one of: NONE, WALK, JUMPWALK, MINIMIZE, JUMPMINI:
- NONE - no change in the procedure
- WALK - switch to Monte-Carlo steps (the default);
- MINIMIZE - switch to gradient-free minimization of the latest accepted force-field;
- JUMPWALK - take the best force-field so far and start the Monte-Carlo procedure from there;
- JUMPMINI - take the best force-field so far and minimize it.
- ScaleFactor - change the current step size corresponding to the *mcstep* control parameter
- ActiveParameterFraction - set the fraction of force-field parameters changed at each step (*mcacpf*)
- deltaBeta - change the current value of the *mcdbet* control parameter
- BetaScaling - change the current value of the *mcbzca* control parameter
- ScaleParSpace - change the current value of the *mcscps* control parameter





## GRAND CANONICAL MONTE CARLO (GCMC)

### 6.1 General info

#### About Monte Carlo / the Grand Canonical Ensemble

It is best to read a bit about Monte Carlo and ensembles before working with the GCMC code. Almost every book or review text on molecular simulations will do, for example: Frenkel D, Smit B. *Understanding molecular simulation: from algorithms to applications*. Academic Press; 2002. 672 p.

Wikipedia also has some pages of interest:

- [http://en.wikipedia.org/wiki/Monte\\_Carlo\\_method](http://en.wikipedia.org/wiki/Monte_Carlo_method)
- [http://en.wikipedia.org/wiki/Grand\\_canonical\\_ensemble](http://en.wikipedia.org/wiki/Grand_canonical_ensemble)

It is important to note that this method heavily relies on random numbers, and simulations are thus non-repeatable in detail, but should converge to the same answer.

#### About the Reaxff GCMC code

The GCMC code for reaxff was originally developed by Thomas Senftle, working as a Graduate Student at Penn State University under the supervision of Dr. Adri van Duin. The original version was a wrapper code that called an external executable to perform the reaxff minimization step and energy calculation, and relied on file modification and parsing to steer the reaxff code and get the results back.

A rewrite of the code, made by Hans van Schoot (SCM) in close collaboration with Thomas Senftle, is now available in the ADF package. The rewrite directly integrates into the ADF-ReaxFF code, solving performance issues of the original code by removing the calling overhead of the reaxff executable and the relatively slow file management. It also merged several modifications of the original code to support the usage of whole molecules for Monte Carlo moves, and supports the usage of multiple atom/molecule types during the simulation. Other improvements were made on the input options, the accessible volume calculation, the MC acceptance prefactor calculation and the writing of logfiles.

The relevant papers are:

Thomas P. Senftle, Randall J. Meyer, Michael J. Janik and Adri C.T. van Duin, *Development of a ReaxFF potential for Pd/O and application to palladium oxide formation*, *J. Chem. Phys.* 139, 044109 (2013) (<http://dx.doi.org/10.1063/1.4815820>)

Thomas P. Senftle, Adri C.T. van Duin, Michael J. Janik, *Determining in situ phases of a nanoparticle catalyst via grand canonical Monte Carlo simulations with the ReaxFF potential*, *Catalysis Communications* volume 52, 5 July 2014, Pages 72–77 (<http://dx.doi.org/10.1016/j.catcom.2013.12.001>)

## 6.2 Input

A worked out GCMC exercise is available from a 2-day ReaxFF workshop (<https://www.scm.com/adf-modeling-suite/adf-hands-on-workshops/advanced-2-day-reaxff-workshop/>).

### Overview

The GCMC code in ADF-ReaxFF needs the following input files to run:

- control\_MC : The GCMC control file, which holds MC settings and the atoms/molecules to insert/move/delete
- control : A reaxff control file, in which only a small number of parameters is of interest
- ffield : A standard reaxff forcefield file
- geo : A geometry file, preferably in biograph format (code not yet tested with xyz)
- iopt : Text file that should only contain a “5” (without the quotes)
- insertData\_MC : (optional file) Table used when restarting GCMC simulations

Also, the current version of the GCMC code can only run in serial, so please set the NSCM environment variable to 1 (type “export NSCM=1” (without quotes) in the shell before starting a GCMC reaxff run).

### the control\_MC file

Lines in the control\_MC file that start with ! or # will be ignored, so those can be used for comments. Empty lines are also ignored, so feel free to leave some in the file. Lines with keywords should have their value in the first 8 columns, followed by a couple of spaces (at least 1), followed by the 6-character keyword. The order is free, except for the nmols keyword, which should be the last one. The nmols keyword signals the parser that the next section of control\_MC will define X new MC Molecule Types.

This is an example for the control\_MC file:

```
! GCMC control file example
  0  iensmb !select MC ensemble (0=Mu-NVT with fixed volume, 1=Mu-NPT with
↳variable volume)
 5000 niter !number of MC iterations to do this simulation
  0  nstart !start the iteration counter with an offset, usefull for restarts to
↳avoid double files
 300.0 mctemp !Temperature of the simulation, affects acceptance rate for steps
↳that increase the energy
  0.0 mcpres !NPT pressure in GPa (set to zero for incompressible solid systems
↳unless at very high pressures)
  3.0 rmaxpl !Max radius for atom placement on insert/displace move
  1.2 rminpl !Min radius for atom placement on insert/displace move
 2000 nmctry !Maximum number of trials allowed when inserting or moving a
↳molecule. If the
!           ! rmaxpl and rminpl variables are very strict, this number needs to
↳be large
  1  igcfac !include GC prefactor in probabilities? 0 = no 1 = yes
  0  ivol  !select MC volume calculation technique:
!           ! 0: vvacu needed! volume = total volume - occupied volume -
↳specified vacuum volume (vvacu)
!           ! 1:           volume = total cell volume
!           ! 2: vacc needed! volume = specified accessible volume (vacc)
!           ! 3:           volume = total cell volume - occupied volume
!           ! 4: vacc needed! volume = specified accessible volume (vacc) -
↳occupied volume
 435.0 vacc  !if ivol=2 or ivol=4, specify Vacc in angrstoms^3
  0.0 vvacu !if ivol=0 specify non-accessible (vacuum) volume Vvacu in angrstoms^
↳3
```

```

0.25  ivlim  !volume change limit (value between 0 and 1, Vnew =
↳ ((1+ivlim)*V1)
    1  resopt !write restart files: 0=no, 1=yes
    1  resfrq !frequency of writing restart files (MC code only writes files if
↳the MC move is accepted)
    0  debug  !print debug output if set to 1, print even more debug output when
↳set to 2
    5  nmols  !Number of MC molecule types, must match the number of molecule
↳blocks that follow!
!
! Molecule Specific Data: C2H2 example
!   This part is fixed format!
!   We need cmpot on line 1,
!   possibly followed by the noinsr on line two,
!   and forced to be ended with nmatom on line 2 or 3, followed by nmatom lines of
↳coordinates.
! the coordinates are FIXED FORMAT! (24d.15,1x,A2) x,y,z (24 wide, 15 after decimal),
↳1 space, 2chars symbol)
-75.00  cmpot  !chemical potential of molecule
    4  nmatom  !number of atoms in molecule
        12.1804800000000000      0.4216960000000000      1.3166890000000000 C
        13.1247310000000000      0.3769020000000000      0.5683600000000000 C
        11.3494750000000000      0.4595600000000000      1.9882080000000000 H
        13.9573140000000000      0.3358430000000000      -0.1010000000000000 H

!Molecule Specific Data: C2H4 example
-75.00  cmpot  !chemical potential of molecule
    6  nmatom  !number of atoms in molecule
        13.9892220000000000      0.4053910000000000      1.0001500000000000 C
        13.3167840000000000      0.3996460000000000      0.8857950000000000 C
        11.4945130000000000      0.4618370000000000      1.9706120000000000 H
        11.3352190000000000      0.3535770000000000      0.1295810000000000 H
        13.8117010000000000      0.3402240000000000      -0.0840000000000000 H
        13.9705610000000000      0.4533250000000000      1.7562360000000000 H

!Molecule Specific Data: H2O Example
-75.00  cmpot  !chemical potential of molecule
    1  noinsr  !setting this to 1 disables insert/deletion moves. If it is set to
↳1 for all types, the ensemble becomes NVT/NPT
    3  nmatom  !number of atoms in molecule
        39.9967200000000000      40.7476600000000000      40.5122100000000000 H
        40.0002100000000000      39.9995200000000000      39.9347300000000000 O
        40.0000300000000000      39.2598800000000000      40.5237000000000000 H

!Molecule Specific Data: H2 Example
-75.00  cmpot  !chemical potential of molecule
    2  nmatom  !number of atoms in molecule
        5.0258120000000000      0.0000000000000000      0.0000000000000000 H
        5.7741880000000000      0.0000000000000000      0.0000000000000000 H

!Molecule Specific Data: Single atom example
-75.00  cmpot  !chemical potential of molecule
    1  nmatom  !number of atoms in molecule
        0.0000000000000000      0.0000000000000000      0.0000000000000000 H

```

The Molecule Specific Data blocks define the molecules (or atoms) that can be inserted/moved/deleted with the MC code. The atoms named here should of course be in the forcefield files, and the coordinates should form a reasonable structure. The MC code uses these coordinates during the insertion step by giving them a random rotation, followed

by a random translation to generate a random position of the molecule inside the box. Currently, there is no check to make sure the molecule stays inside the boundaries of the box, the code only checks that the `rmaxpl/rminpl` values are satisfied. If you plan on inserting large molecules, make sure there is enough room in the `rmaxpl` value, otherwise the code will stop with an error message.

### The chemical potential (`cmpot`) keyword

The `cmpot` keyword sets the chemical potential of the molecule (or atom) reservoir, and is employed when calculating the Boltzmann accept/reject criteria after a MC move is executed. This value can be derived from first principles using statistical mechanics, or equivalently, it can be determined from thermochemical tables available in literature sources.

For example, the proper chemical potential for a GCMC simulation in which single oxygen atoms are exchanged with a reservoir of O<sub>2</sub> gas, should equal 1/2 the chemical potential of O<sub>2</sub> at the temperature and pressure of the reservoir:

$$\text{cmpot} = \text{Mu}_O(T,P) = 1/2 * \text{Mu}_{O_2}(T,P) = 1/2 * [\text{Mu}_{\text{ref}}(T,P_{\text{ref}}) + kT * \text{Log}(P/P_{\text{ref}}) - E_{\text{diss}}]$$

where the reference chemical potential [ $\text{Mu}_{\text{ref}}(T,P_{\text{ref}})$ ] is the experimentally determined chemical potential of O<sub>2</sub> at T and  $P_{\text{ref}}$ ,  $kT * \text{Log}(P/P_{\text{ref}})$  is the pressure correction to the free energy, and  $E_{\text{diss}}$  is the dissociation energy of the O<sub>2</sub> molecule.

### The no insert (`noinrs`) keyword

The `noinrs` keyword tells the GCMC code to keep the number of molecules/atoms of this type fixed. It will thus disable Insert/Delete moves on this type, meaning it can only do a displacement move, or volume change move (if the `iensmb` keyword is set to 1).

### the control file

The control file is a regular reaxff control file and it influences the minimization step after an MC trial move. Because of this, only a small number of the reaxff keywords are used during the GCMC simulation.

An example of the control file:

```
# some of the parameters that influence the minimization step in the GCMC code
  1 icentr      Put the center of mass at the center of the cube
  1 igeofo      0:xyz-input geometry 1: Biograf input geometry 2: xmol-input
↪geometry
2.50000 endmm  End point criterium for MM energy minimisation
  500 imaxit    Maximum number of iterations
  0 icelop     Optimize cell parameters 0=no 1=yes
1.00050 celopt Cell parameter change
  0 imaxmo     In this case: 0: POLAK_RIBIERE Conj.Grad method, 1: Limited-memory
↪BFGS method
```

The code has been tested with various `imaxit` and `endmm` values, the other options have not been fully tested. Other reaxff keywords might also influence the minimization procedure, but those are best left to their default settings

### the ffield file

The `ffield` file should be a normal reaxff forcefield file, as described in the reaxff documentation by A. van Duin (visit the documentation section on the SCM website to obtain this document).

### the geo file

The GCMC code has been tested with biograph input files, but other input formats might work. The details of this file are also described in the original reaxff documentation by van Duin.

### the iopt file

The `iopt` file is a text file with a single digit inside that selects the execution mode of the reaxff code. To run the GCMC code, this file should contain a "5" (without the quotes).

### the insertData\_MC file

The GCMC code can insert multiple atom/molecule types in a single simulation, so it needs to keep track of what atom belongs to which insert. This information is automatically stored and updated when insertion/deletion/moving of atoms or molecules during the simulation, but is by default unknown of the atoms of the starting geometry. The GCMC code will therefore by default not modify the atoms in the original input in the MC trial moves (keep in mind that they can move around during the minimization step). The insertData\_MC file can be used to tell the GCMC code what atoms in the geo file belong to which molecule.

An example of the insertData\_MC file:

#	atomNumber	MCInsMolType	MCInsertNmbr
	30	1	1
	40	2	1
	46	2	1
	47	1	2
	48	1	3

This example specifies 4 molecules/atoms that are modifiable by the GCMC code, belonging to 2 different GCMC molecules/atoms that are defined in the control\_MC file. The first “molecule” in the control\_MC file should thus consist of a single atom (if this doesn’t match, the code will most likely crash!). It was inserted three times (atom 30, 47 and 48) The second molecule has two atoms, and was inserted once.

The atoms do not have a fixed order, and not all atoms have to be defined. If an atom is not appointed to a certain MCInsMolType and MCInsertNmbr, it will simply not be modified during the MC moves. The insertData\_MCXXXXXX files generated by the restart option of the code can be directly used as valid insertData\_MC files, just remove the digits from the filename and replace the geo file with the corresponding geo\_MCXXXXXX file.

## 6.3 Output

### Overview

The GCMC code writes a couple of output files, each described in this section. It also produces a number of reaxff output files, and some of these are described in the original reaxff documentation by van Duin. Keep in mind that these files might not provide a complete or correct picture of the simulation, as they could also contain data originating from rejected MC trial moves.

#### geo\_MCXXXXXX

This file is generated every X accepted MC moves and contains the current geometry of the system in biograph format (X is set with the resfrq keyword in the control\_MC file).

#### insertData\_MCXXXXXX

This file contains a table of all the atoms in the system with their MC Molecule Type and MC Insert Number. This data can be used to map atoms to an inserted molecule, and is needed if you want to restart your calculation from an accepted MC step. The table contains -1 values for atoms that were in the original input and did not get a manually assigned MCInsert Molecule Type and MC Insert Number, the GCMC code will not modify these atoms during the MC steps.

Also see the section on insertData\_MC file.

#### MCstats

The MCstats file is a logfile that contains the statistics of the MC simulation. The GCMC code writes a single line to it after every MC step, containing the number of: Tried MC moves (tried), Accepted MC moves (accept), Rejected MC moves (reject), Accepted Insertion/Deletion/Moving/Volume change MC moves (addAcc/delAcc/mvAcc/volAcc), Rejected Insertion/Deletion/Moving/Volume change MC moves (addRej/delRej/mvRej/volRej)

An example of the MCstats file:

tried	accept	reject	addAcc	delAcc	mvAcc	volAcc	addRej	delRej	mvRej	volRej
0	1	0	1	0	0	0	0	0	0	0
1	1	1	1	0	0	0	0	0	1	0
2	1	2	1	0	0	0	0	0	2	0
3	1	3	1	0	0	0	0	1	2	0
4	1	4	1	0	0	0	1	1	2	0
5	1	5	1	0	0	0	1	1	3	0
6	1	6	1	0	0	0	1	2	3	0
7	1	7	1	0	0	0	1	3	3	0
8	1	8	1	0	0	0	1	3	4	0
9	1	9	1	0	0	0	1	4	4	0
10	1	10	1	0	0	0	1	4	5	0
11	2	10	2	0	0	0	1	4	5	0
12	3	10	3	0	0	0	1	4	5	0

### Elog

The Elog file contains the Volume and energies of the accepted MC steps. The energies in this logfile are the pure ReaxFF energy of the system (RxFFEnergy) and the MC corrected energy, which is used in determining if the step should be accepted or not (see the section on calculating energies for details).

An example of the Elog file:

Iteration	Naccepted	Volume	MC Energy	RxFFEnergy
0	1	15625.00	-3098.88	-3179.88
2	2	15625.00	-3107.92	-3269.92
3	3	15625.00	-3130.13	-3373.13
4	4	15625.00	-3160.05	-3484.05
6	5	15625.00	-3169.77	-3493.77
11	6	15625.00	-3200.13	-3605.13

### reaxout.kf

This is the binary logfile generated by the GCMC code. Its contents can be viewed with the KFBrowser utility, or it can be loaded into ADFMovie to view the geometries in the file. Only the data of successful MC moves is written to this file.

## 6.4 Code Details

### Overview

The GCMC code will perform niter (control\_MC file option) Grand Canonical Monte Carlo trial moves, and accept or reject them based on the Energy produced by the ReaxFF minimization step of the trial geometry. The Monte Carlo algorithm will always accept a step if it results in a decrease of the energy, and accept steps that go up in energy with a probability. This section will give some details about how the code works.

### MC Moves (Insert/Delete/Move/Volume)

The GCMC code currently supports 4 types of MC Moves: Insert, Delete, Move (displace), Volume change. The first three moves always change a whole “molecule” of the system, as defined in the control\_MC file (a molecule can of course contain only a single atom). Every MC iteration selects one MC Molecule Type from the defined molecules in control\_MC at random, followed by a random MC Move (unless there are no molecules of the type in the system, in that case it will do an insert move).

The Insert and Displace (move) MC Moves will generate a random rotation and position for the molecule, and then check if the random positions are within the “RminPI” and “RmaxPI” boundaries (this means no atom in the molecule can be closer to any atom currently in the system than “RminPI”, and it should be within “RmaxPI” distance to an

atom in the system). If the conditions are not satisfied, a new set of coordinates is generated and the code checks again. This is repeated a maximum number of “nmctry” times before stopping with an error.

The volume change is controlled by the “ivlim” variable in control\_MC. The ivlim sets the volume change limit, and it should be a value between 0 and 1. The new volume will be calculated like this:  $V_{\text{new}} = (1 + \text{ivlim}) * V_{\text{old}}$ .

### Calculating energies

Because the GCMC simulation adds and deletes atoms or molecules during the runtime, it cannot directly compare the ReaxFF energies for the MC acceptance criteria: inserting a molecule will usually lower the total energy of the system, causing the MC to always accept it, and always reject a deletion. To balance this out, the GCMC code calculates a “corrected” MC energy to compare the trial reaxFF energy with, consisting of the previously accepted ReaxFF energy + the chemical potential (cmpot in control\_MC) for the inserted molecule, or the ReaxFF energy - the chemical potential for the deleted molecule. The volume change energy is also corrected, using the following formula:

$$E_{\text{MC\_Corr}} = E_{\text{reaxff\_last\_accept}} - (\text{Pressure} * 0.1439 * (\text{newV} - \text{oldV})) + ((1.0/\beta) * n_{\text{InsertedMols}} * \log(\text{newV}_{\text{avail}}/\text{oldV}_{\text{avail}}))$$

where newVavail and oldVavail are calculated from the MC available volume (see the section calculating volumes).

### Calculating volumes

The GCMC code can calculate the available volume in a couple of different ways, depending on the ivol setting in control\_MC:

- ivol = 0: volume = total volume - occupied volume - specified vacuum volume (vvacu)
- ivol = 1: volume = total cell volume
- ivol = 2: volume = specified accessible volume (vacc)
- ivol = 3: volume = total cell volume - occupied volume
- ivol = 4: volume = specified accessible volume (vacc) - occupied volume

Where the occupied volume is calculated by summing up the volumes of the atoms in the geo file that are not specified to be part of an MC type molecule. The volume of an atom is calculated using the average of the covalent atomic radius and the vd Waals radius of the atom, which are found in the reaxff forcefield file (ffield).

the vacc and vvacu options can be specified in the control\_MC file to get a more accurate available volume.

### Acceptance criteria

An MC move is always accepted if the reaxff energy is lower than the corrected MC energy of the last accepted MC move, or if the energy increase is small enough. If the new energy is higher, the code generates a random number between 0 and 1, and accepts the move if the random number is bigger than:

$$\text{prob} = \text{preFactor} * \exp(-\text{Beta} * \text{deltaE})$$

Where the prefactor is calculated (for insert and delete moves) using the deBroglie wavelength of the inserted molecules, the number of inserted molecules and the available MC volume of the system.

## 6.5 Tutorial: Discharge voltages

**Note:** This tutorial requires the [ADF development version](https://www.scm.com/support/downloads/development-snapshots/) (https://www.scm.com/support/downloads/development-snapshots/) with a revision number greater than r62841.

### Overview

This advanced ReaxFF tutorial will teach you how to calculate the discharge voltage profile of a LiS battery.



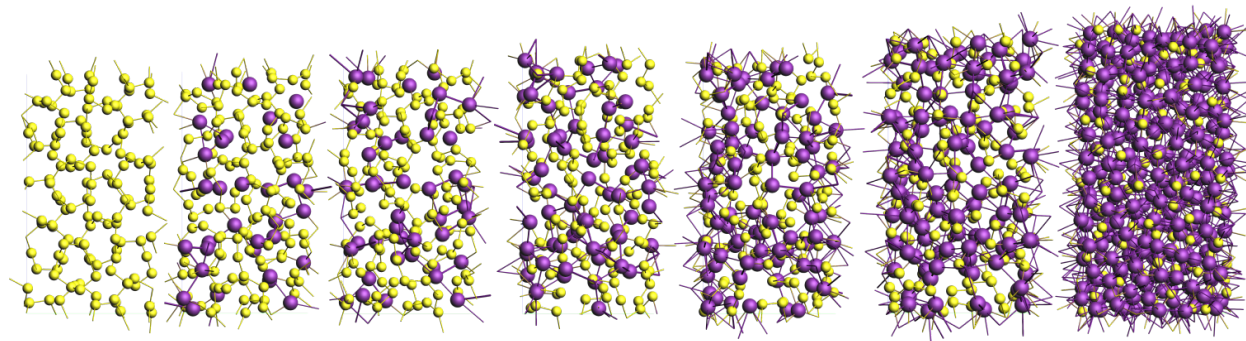
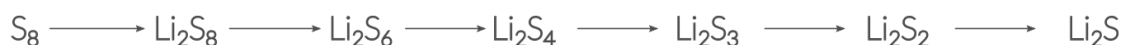
Contents:

- Importing a CIF file from an external database and equilibrating the structure
- Calculating the chemical potential for Li
- Setting up a grand canonical monte carlo (GCMC) simulation w. ReaxFF
- Results: How to calculate the discharge voltage profiles.

If you are not familiar with using the GUI yet, you might take a look at the [ReaxFF GUI tutorials](https://www.scm.com/doc/Tutorials/ReaxFF/ReaxFF-GUI_tutorials.html#reaxff-gui-tutorials) ([https://www.scm.com/doc/Tutorials/ReaxFF/ReaxFF-GUI\\_tutorials.html#reaxff-gui-tutorials](https://www.scm.com/doc/Tutorials/ReaxFF/ReaxFF-GUI_tutorials.html#reaxff-gui-tutorials)) before continuing.

## The System

This tutorial uses a small alpha-sulfur system consisting of 128 atoms. Both the system and the workflow presented here are originally described in the publication “[ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials](https://doi.org/10.1039/C4CP04532G)” by M.M.Islam et al. (<https://doi.org/10.1039/C4CP04532G>)



The discharge process is simulated using ReaxFF in a grand canonical monte carlo scheme. Volume changes upon lithiation are accounted for by using an  $N_SPT-\mu_{Li}$  scheme. The discharge voltage can be calculated from the total energies of the lithiated compounds.

### 1. Importing the Sulfur( $\alpha$ ) crystal structure

The crystal structure can be directly imported from a CIF file (<http://ruff.geo.arizona.edu/AMS/download.php?id=11560.cif&down=cif>). There are several resources for crystallographic data available online and you can choose according to your liking. Here we use a structure of  $\text{S}_8$  alpha sulfur from the [American Mineralogist Crystal Structure Database](http://ruff.geo.arizona.edu/AMS/amcsd.php) (<http://ruff.geo.arizona.edu/AMS/amcsd.php>).

The downloaded CIF can directly be imported into ADFinput:

```
File → Import Coordinates
Edit → Crystal → Map atoms to (0..1)
View → Periodic → Show lattice vectors
```

The latter two steps map the coordinates into the ReaxFF unit cell and display the lattice vectors.

Before adding any Li-ions to the system, we need to relax the structure using a geometry and cell optimization, i.e. including the optimization of lattice vectors.

---

**Tip:** Often we find that running a couple of hundred steps NPT dynamics at low temperature and 0.0 pressure using a small timestep is sufficient as a relaxation or at least speed up a subsequent geometry optimization significantly.

---

With the current system we can run a geometry and cell optimization directly:



Select the **LiS.ff** force field  
 Select **Task** → **Geometry Optimization**  
 Switch to **Details** → **Geometry Optimization**  
 Select **Conjugate Gradient**  
 Set the max. steps to 5000  
 Select **Cell Optimization** → **Full Cell**

Save and run the calculation to yield a total energy of

$$E_S = -8535.99 \text{ kcal/mol}$$

## 2. Importing the Sulfur( $\alpha$ ) crystal structure

Following the literature approach, we fix the external chemical potential of Li at the total energy of a single lithium atom in body-centered cubic lithium. The structure of bcc Lithium can be created easily via the crystal builder from within ADFinput:

**Edit** → **Crystal** → **Cubic** → **bcc**  
**Select Li from the Presets and click OK**  
**Edit** → **Crystal** → **Generate Supercell**  
 Enter 8, 8, 8 on the diagonal to create an 8x8x8 supercell (512 atoms)  
**Edit** → **Crystal** → **Map atoms to (0..1)**

Optimize the resulting structure and lattice using the same settings as with the sulfur.

After the optimization has finished successful, the chemical potential is calculated as the total energy / number of atoms.

---

**Note:** The exact value depends to some minor extent on the chosen force field and for consistency one should always use the value predicted by the force field at use.

---

Throughout this recipe the LiS.ff is used and the chemical potential of Li will be fixed at

$$\mu_{Li} = -37.70 \text{ kcal/mol}$$

## 3. Setting up the GCMC calculation

GCMC calculations are quite sensitive to the chosen settings. The main reason being the interplay of comparing small energy differences in the GCMC acceptance criteria and the optimization procedure carried out after each MC-trial move.

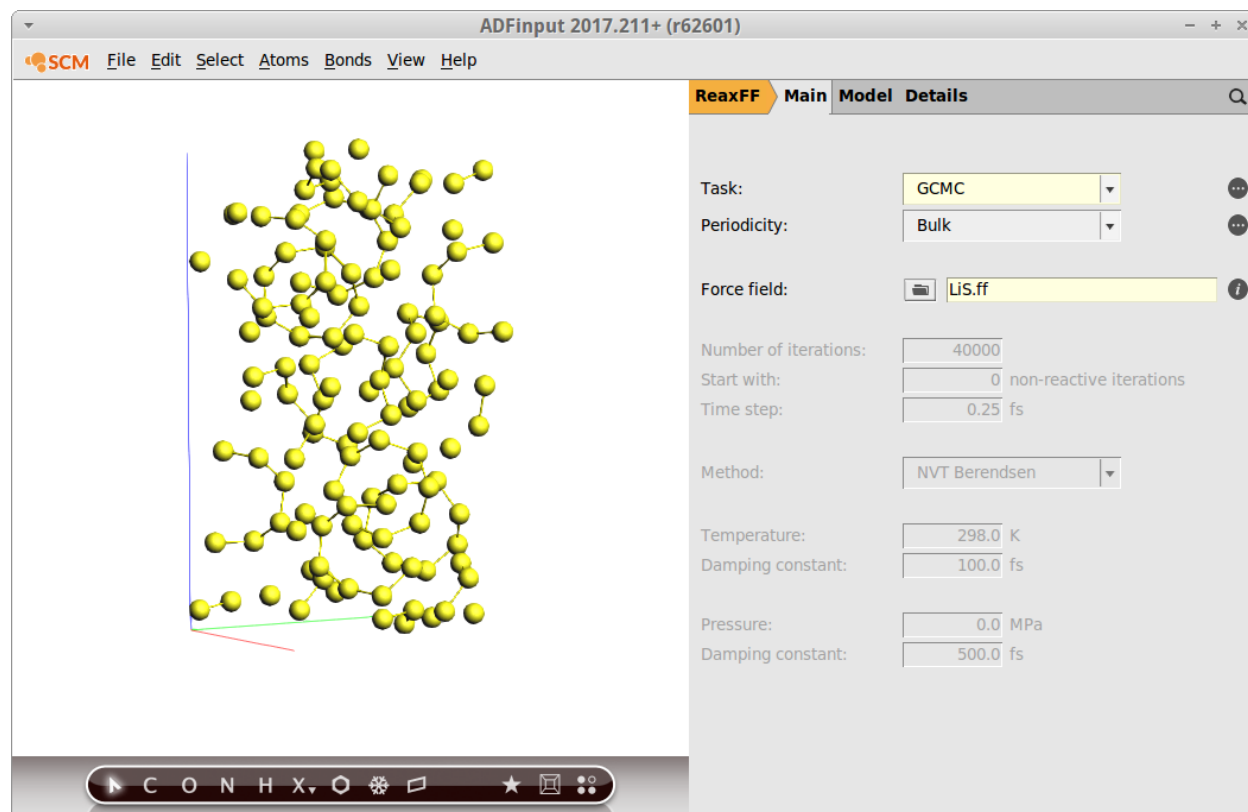
---

**Note:** Its advised to try different optimizer settings (max. steps, convergence criteria, etc...). The GCMC settings are documented online ([here](#)).

---

The [ADF development version](https://www.scm.com/support/downloads/development-snapshots/) (>= r62841) comes GUI support for GCMC calculations. We will be using the GUI in this tutorial but the same calculation can be run from the commandline as well.

Our previously optimized S<sub>8</sub> structure will serve as the system:



**Task** → **GCMC**

Switch to the GCMC panel: **Model** → **GCMC**

Select **MC ensemble** →  $\mu$ **PT**

This will be enough steps to converge the current system. However, this value is not known beforehand and one might want to choose a larger number of iterations for larger systems.

Set **Temperature** to 300

Add molecules between 1.2 and 6.0 Å

These fields correspond to the  $R_{max}$  and  $R_{min}$  values in the GCMC input. You can try different values here. As a complete empirical rule of thumb: setting  $R_{min}$  to roughly  $\frac{1}{2}$  of the shortest expected bond and  $R_{max}$  approx. half of the shortest lattice vector seems a good starting point.

**Max. tries** → 3000

The number of attempted tries must be sufficiently large. If this is not the case, the calculation will abort with an error message stating that number of max tries was exceeded.

#### **Molecule to add**

Press the button labelled +

Enter `Li` as the name

The name is generic, you will still need to draw a Lithium atom into the window labelled “Li” in the molecule view to the left. After placing the Li-atom, select it place it in the middle of the unit cell as follows

Edit → Crystal → Set(0.5,0.5,0.5)

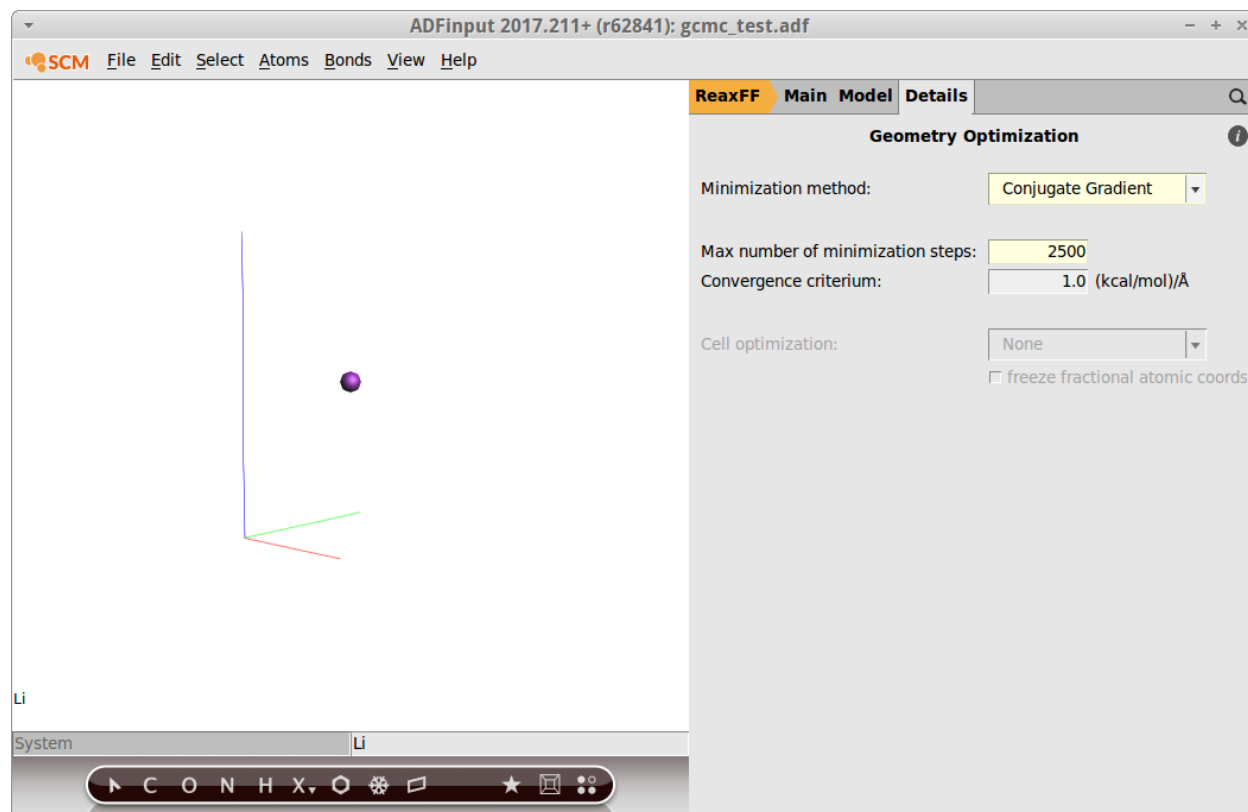
The screenshot shows the ADFinput software interface. The main window displays a 3D coordinate system with a single purple sphere representing the Li atom. The right-hand panel is titled "GCMC" and contains various configuration options. Under "Minimization details", there is a button with three dots. Below that, a table lists the molecule to add and its chemical potential.

+	Molecule to add	$\mu$ (kcal/mol)
-	Li	-37.70

The optimizer settings can be found by clicking on the button labelled "..." next to **Minimization details**. Remember that the optimizer settings are most crucial for the GCMC algorithm:

Select **Minimization method** → **Conjugate Gradient**

Set **Max. number of steps** to 2500



Save your changes and run the calculation. The initial stages of the calculation are reached quite fast and the progress can be followed in ADFmovie. However, it will typically take a bit less than one day until convergence.

#### 4. GCMC Troubleshoot

No MC-moves are accepted:

- Check if you set the correct chemical potential (remember to use the one calculated with your force field!)
- Tighten the convergence criteria for the optimization
- Change  $R_{max}$  and  $R_{min}$  settings
- Try to optimize the system (here: the sulfur structure) with tighter optimization settings
- Try a different force field

The calculation takes a lot of time:

- Loosen the convergence criteria, e.g. less steps and a lower convergence criterium
- The obvious: Try a smaller system.

#### 5. Results

The discharge voltage profiles can be calculated as a function of Li intercalation content from

$$V(x) = -\frac{G_{Li_x} - x \cdot G_{Li} - G_S}{x}$$

where  $G$  denotes the Gibbs free energy and  $x$  the concentration of Li-ions. The enthalpic (PT) and entropic (TS) contributions can be neglected and thus the Gibbs free energy replaced by the ground state energy.

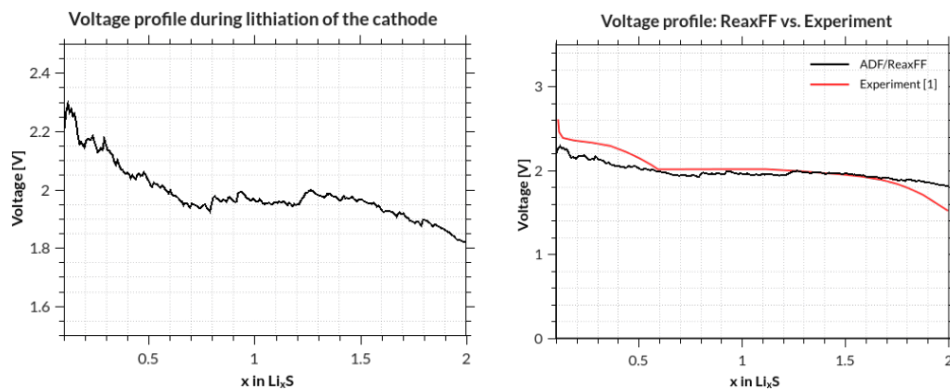
In this case and many other cases of non-standard trajectory analysis, writing a short Python script using the [PLAMS](https://www.scm.com/doc/plams/started.html#getting-started) (<https://www.scm.com/doc/plams/started.html#getting-started>) library is the most efficient way to obtain results. Re-

member there is no need to take any further action than writing the script: Both Python and PLAMS are shipped with every copy of ADF/ReaxFF.

The script called `LiVoltageProfile.py` is available [here](https://downloads.scm.com/distr/LiVoltageProfile.py) (<https://downloads.scm.com/distr/LiVoltageProfile.py>) and can be run as follows from the command line:

```
$ADFBIN/startpython LiVoltageProfile.py gcmc_test.rxkf
```

assuming that your trajectory was called `gcmc_test.rxkf` and that you used the same system and force field as explained in this recipe. The results are written to a file called `voltage_profile.out`:



Lit.:

[1] M. M. Islam, A. Ostadhossein, O. Borodin, A. Todd Yeates, W. W. Tipton, R. G. Hennig, N. Kumar and A. C. T. van Duin *ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials*, *Phys. Chem. Chem. Phys.* **17**, 3383-3393 (2015). (<https://doi.org/10.1039/C4CP04532G>)



## FORCE-BIAS MONTE CARLO (FBMC)

The Uniform-acceptance force-bias Monte Carlo (fbMC) method ([Phys. Rev. B 85, 134301 \(2012\)](https://doi.org/10.1103/PhysRevB.85.134301)) has been implemented in ADF ReaxFF by the group of Erik Neyts.

Usually, ReaxFF optimizations are alternated with fbMC steps to accelerate events such as reactions. The acceleration (MC step) is controlled by the temperature and maximum displacement, which should be balanced to keep close to the real dynamics. fbMC does not scale time uniformly ([J. Chem. Phys. 141, 204104 \(2014\)](http://dx.doi.org/10.1063/1.4902136)). Diffusion coefficients and reaction rates should probably use quartic mass scaling.

fbMC mass scaling can be set. It defaults to quadratic scaling as in the original fbMC implementation. Setting *imcroo* to 4 would mean quartic mass scaling.

### Input keywords

These keywords should be set at the end of the *control* file. fbMC control parameters can also be set in the GUI, except for *imcroo*.

- *drmax* – maximum displacement
- *imcfrq* – frequency of fbMC steps
- *imcstp* – number of fbMC steps
- *imcroo* – mass scaling (defaults to 2, 4 is recommended as per the Bal & Neyts paper)

A worked out example for fbMC versus unaccelerated ReaxFF MD for healing graphene has been made for the [2-day ReaxFF workshop](https://www.scm.com/adf-modeling-suite/adf-hands-on-workshops/advanced-2-day-reaxff-workshop/).





## THE MOLECULE GUN

The molecule gun allows you to “shoot” (add with velocity) a molecule into the simulation box. Molecules can be continuously added to the simulation or only once. The initial position as well as the initial velocity can be pre-set or random w.r.t. to all or a selection of X,Y,Z-components. Possible applications of the molecule gun include e.g. the simulation of enforced collisions or deposition processes on surfaces.

**See also:**

**Mol. Gun GUI tutorial** ([https://www.scm.com/doc/Tutorials/ReaxFF/Bouncing\\_a\\_buckyball.html#the-molecule-gun](https://www.scm.com/doc/Tutorials/ReaxFF/Bouncing_a_buckyball.html#the-molecule-gun))

The molecule gun requires an additional input file called **addmol.bgf**. It contains the geometry of the particle to be shot in BGF format and some additional keywords.

The following keywords may be specified in the **addmol.bgf** file:

**Input Keywords**

- *FREQADD* – Add new molecule every N-th step but not before the iteration specified in FIRSTADD
- *FIRSTADD* – Add the first molecule at iteration N
- *VELADD* – Velocity of the added molecule: 1 - random, 2 - specified in the addmol.vel file, 3 - via a temperature specified with *TADDMOL*
- *STARTX* – The initial X coordinate of the added molecule, random if not specified
- *STARTY* – The initial Y coordinate of the added molecule, random if not specified
- *STARTZ* – The initial Z coordinate of the added molecule, random if not specified
- *ADDIST* – Minimum distance from the molecule to other atoms for successful addition
- *NATTEMPT* – The program will try to add a molecule N times until the ADDIST criterion is met
- *TADDMOL* – for VELADD=1|3: temperature for the velocity of the molecule as a whole
- *ROTATE* – The molecule is rotated randomly before being added
- *SIGMAX* – sigma parameter for the Gauss distribution of the initial X coordinate around STARTX
- *SIGMAY* – sigma parameter for the Gauss distribution of the initial Y coordinate around STARTY
- *SIGMAZ* – sigma parameter for the Gauss distribution of the initial Z coordinate around STARTZ
- *VELXYZ* (V<sub>x</sub> V<sub>y</sub> V<sub>z</sub>) – for VELADD=3: the direction vector for the initial velocity of the added molecule
- *SIGMAT* – for VELADD=1|3: standard deviation for TADDMOL
- *TDISPER* – for VELADD=3: each atom’s velocity is modified with  $V_{\{x,y,z\}} = \sqrt{RT/m} * \text{random\_normal}(0,1)$

**Example**

The following example **addmol.bgf** file will create one carbon atom every 1000th iteration starting from iteration 500. The added atom will have an initial temperature of 800K and will initially move in the positive direction along the Z axis.

```
BIOGRF 200
DESCRP C
REMARK Created by ADFinput
VELADD 3
FIRSTADD 500
FREQADD 1000
STARTX 1.671997104
STARTY -4.00486678
STARTZ -0.3259654382
ROTATE 1
TADDMOL 800
VELXYZ 0.0 0.0 5.0
HETATM 1 C 1.67200 -4.00487 -0.32597 C 1 1 0.0
END
```

---

**Tip:** Use the GUI to [setup a molecule gun](https://www.scm.com/doc/Tutorials/ReaxFF/Bouncing_a_buckyball.html#the-molecule-gun) (https://www.scm.com/doc/Tutorials/ReaxFF/Bouncing\_a\_buckyball.html#the-molecule-gun) calculation and edit the .run file created by the GUI to minimize typos. The section *addmol.bgf* is found at the end of the run file just before the *control* section.

---

### Changes with respect to the original reac program

It is possible to add some randomness both to the pre-set position and to the velocity: the SIGMA{X,Y,Z} keywords specify a standard deviation value for the Gauss distribution around the START{X,Y,Z} values, respectively. If "ROTATE 1" is specified, the molecule will be rotated randomly around its geometric center before being added to the system.

A VELADD=3 option has been added. With this option, it is possible to specify the velocity vector's direction via VELXYZ. This vector is normalized so the exact magnitude of its components does not matter. The magnitude of the velocity along this vector is determined by the TADDMOL and SIGMAT parameters as  $\sqrt{3nRT/M}$ , where  $T=TADDMOL + SIGMAT * \text{random\_normal}(0,1)$ , n - number of atoms in the molecule, R - gas constant, M - molar mass. Additionally, the velocity of each atom may be modified with a random component based on the temperature specified by the TDISPER keyword. On average, the total temperature of the added molecules should be close to TADDMOL+TDISPER.

Molecules will never be added before the step specified by the FIRSTADD keyword. Thus, a molecule will always be added at the FIRSTADD step and then at every iteration divisible by FREQADD. If, for example, FIRSTADD=1999 and FREQADD=1000 then the first molecule will be added at iteration 1999, the second at iteration 2000 and then every 1000-th iteration after that.

## TRAVIS: A TRAJECTORY ANALYZER AND VISUALIZER

TRAVIS is a command line C++ program for analyzing and visualizing trajectories from all kinds of Molecular Dynamics or Monte Carlo simulations developed by M. Brehm (*J. Chem. Inf. Model.* 51(8) (2011) (<https://doi.org/10.1021/ci200217w>)). TRAVIS is shipped with the ADF modeling suite from on ADF2017.

The supported input formats of TRAVIS are:

- *xyz*
- *pdb*
- *Imp* (Lammps)
- *HISTORY* (DLPOLY)
- *prmtop/mdcrd* (Amber)

With ADF2017 the analysis of DFTB and ReaxFF trajectories is supported.

---

**Note:** TRAVIS was designed with non-reactive trajectories in mind, thus one needs to make sure that:

- *either* the composition of the target species does not change, e.g. by analyzing only a suitable time-interval or running non-reactive dynamics
  - *or* the analysis does not depend on the detection of a particular species, e.g. the diffusion of (inert) atoms
- 

In order to run a TRAVIS analysis on your trajectory open a shell and navigate to the folder you ran your calculation in. Use the python script **kf\_to\_xyz.py** to convert your trajectory into a TRAVIS-compatible XYZ-format.

Assuming the trajectory is called **traj.rxxf**, run:

```
$ADFBIN/startpython $ADFHOMe/scripting/trajectory_analysis/kf_to_xyz.py
traj.rxxf
```

This step will create a file called **traj\_travis.xyz** that contains the frames in XYZ format plus an additional 5th column containing the ReaxFF atomic charges.

Next, start TRAVIS to enter an interactive dialog:

```
$ADFBIN/travis.exe -p traj_travis.xyz
```

An example of how to use TRAVIS with ReaxFF can be found in the [advanced Li-Batteries ReaxFF tutorial](https://www.scm.com/news/tutorial-li-ion-diffusion-coefficients-reaxff/) (<https://www.scm.com/news/tutorial-li-ion-diffusion-coefficients-reaxff/>).



## OTHER NEW FEATURES AND FIXES

### 10.1 Molecular charges

In order to freeze the total charge of a group of atoms (for example, a molecule) one can add a MOLCHARGE key to the geo file in the BGF format. The format of the key is as follows:

```
MOLCHARGE  n1 n2 q
```

where  $n1$  and  $n2$  specify indices of the first and the last atoms of the molecule and  $q$  is the charge. All atoms between  $n1$  and  $n2$  will be included in the molecule. When specifying the MOLCHARGE key *all* atoms present in the system must be assigned to one of the the molecules. For example, if your system consists of 10 water molecules and the charge of the first of them is constrained to be +1 and the total charge of the system is zero then the following two MOLCHARGE keys must be specified:

```
MOLCHARGE  1  3  1.0  
MOLCHARGE  4 30 -1.0
```

Note: The MOLCHARGE is implemented as a simple constraint in the charge equilibration procedure and it does not take any bonding information into account. This means that specifying molecular charges using the MOLCHARGE key makes sense only if you are sure that the constitution of the molecule will not change during calculation. This is useful, for example, when fitting EEM-related parameters in a force-field.

### 10.2 ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order

The ACKS2 charge equilibration scheme has been implemented following the original paper “ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order” by T. Verstraelen et al. J. Chem. Phys. 138 (2013) 074108.

Using the ACKS2 scheme requires a suitable force-field, which is recognized by “[ acks2 ]” at the start of the first line of force field file (note: the spaces around “acks2” are important!). Besides, the *icharg* parameter in the control file must be set to 7. In addition to the general EEM parameters the ACKS2 scheme needs the general force-field parameter #35 (“Xamp”) and the atomic cut-off parameter #23 (“softcut”).

### 10.3 Correction for torsion angles asymptotics

There is a discontinuity problem for small bond orders in the expression for torsion angles and conjugation contributions  $f(\text{BO})$ . These terms correspond to expressions for  $f_{10}$  (eq. 10b) and  $f_{12}$  (eq. 11b) in the [original ReaxFF paper](#)

(<http://dx.doi.org/10.1021/jp004368u>). The new expression for each term in  $f_{10}$  is  $(1 - e^{-2\lambda_{23}BO^2})$  and in  $f_{12}$  the new expression is  $\sin(\frac{\pi}{3}BO)^4$ . The new expressions ensure correct asymptotic behavior for the dE/dBO for  $BO \rightarrow 0$ . Using this makes geometry optimizations more stable and improves conservation of energy during MD.

The correction can be enabled by setting the tors13 flag in the control file to 1.

## 10.4 LG dispersion

The LG dispersion correction was implemented following the paper “ReaxFF-*lg*: Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials” by Liu et al. *J. Phys. Chem. A*, 2011, 115 (40), pp 11016–11022, <http://dx.doi.org/10.1021/jp201599t>

The LG dispersion correction is turned on when using a suitable forcefield, which is recognized by the “[ *lgDispersion=1* ]” key in the file header.

## 10.5 ChemTraYzer

### 10.5.1 General information

The ChemTraYzer scripts, developed in the [Leonhard group](http://www.ltt.rwth-aachen.de/forschung/molekulare_thermodynamik/molekulare_thermodynamik/project/ChemTraYzer_Modellierung_chemi/) ([http://www.ltt.rwth-aachen.de/forschung/molekulare\\_thermodynamik/molekulare\\_thermodynamik/project/ChemTraYzer\\_Modellierung\\_chemi/](http://www.ltt.rwth-aachen.de/forschung/molekulare_thermodynamik/molekulare_thermodynamik/project/ChemTraYzer_Modellierung_chemi/)) at Aachen University, provide a methodology for deducing quantitative reaction models from reactive molecular dynamics simulations by identifying, quantifying, and evaluating elementary reactions of ReaxFF trajectories.

For usage with ADF’s ReaxFF the scripts have been slightly modified and use RDKit instead of the openbabel-bindings. A GUI-tutorial is available [here](#). The original paper, Automated Discovery of Reaction Pathways, Rate Constants, and Transition States Using Reactive Molecular Dynamics Simulations, can be found [here](http://dx.doi.org/10.1021/acs.jctc.5b00201) (<http://dx.doi.org/10.1021/acs.jctc.5b00201>).

### 10.5.2 Command line execution

#### 1. Open a terminal:

- on Linux: Ctrl+Alt+T usually works, otherwise browse your application menus
- on Windows: double click `adf_command_line.bat` in your ADF installation directory (e.g. `C:/ADF2016.106`), enter ‘sh’ to go to a shell

#### 2. cd into the directory where your trajectories are located with the terminal

#### 3. Assuming your trajectory is called `traj.rxkf`, running ChemTraYzer is a two step procedure

- run the processing step (with default values)

```
$ADFBIN/startpython $ADFHOMe/scripting/chemtrayzer/processing_scm.py traj.rxkf
```

- run the analysis step (with default values)

```
$ADFBIN/startpython $ADFHOMe/scripting/chemtrayzer/analyzing_scm.py traj.rxkf
```

You will probably want to adjust the settings. A list of all available options is shown by calling the scripts without arguments, e.g. `$ADFBIN/startpython $ADFHOMe/scripting/chemtrayzer/analyzing_scm.py`

### 10.5.3 Results

ChemTraYzer creates several output files, the most relevant ones being:

#### **reac.spec.tab**

1st line: indices of the species, e.g. S1;S2;S3;etc...

2nd line: SMILES of the species, e.g. ;C;CC;CCO;CCOO;CO;O;[H];etc...

3rd - end: timestep, counts of the species, e.g. 150;0;0;2;... // step 150, current count of S3 == 2

#### **reac.rate.tab**

1st line: indices of the reactions, e.g. t [steps];R0;R0\*;R1;R1\*; // a "\*" marks the back reaction

2nd line: the reactions formulated with the species indices, e.g. ;S0 + S0 + S0 + S13 -> S65; // see reac.spec.tab

3rd line: the reactions formulated with sum formulas, e.g. CH3 + H -> CH4, etc...

4th -...: timestep;rate constant of the reaction; rate constant of the back reaction; etc...

#### **reac.pic/**

folder containing the 2D structures (if obabel was able to create them) reac.pic/xyz/ xyz files of the species as they first appeared in the trajectory

## 10.6 Repeating the unit cells

A simple way to increase the size of the simulation box is by multiplying it a number of times in the a, b, and c directions. In the ReaxFF program this can be achieved by specifying the *reptx*, *repty*, and *reptz* keys (for the a, b, and c direction, respectively) in the control file. The specified value must be strictly positive and the default is 1 (one) for each of them.





## TROUBLESHOOTING

### 11.1 Geometry optimization

Geometry optimization issues with reaxff are usually caused by the fact that the derivative of the ReaxFF energy function has discontinuities. These discontinuities are often related to the bond order cutoff (cutof2 in the control file, 0.001 by default). This cutoff determines whether a valence or a torsion angle is included in the potential energy evaluation or not, i.e. when at least one of the bonds forming an angle is of order lower than the cutoff then the angle is discarded. Thus, when the order of a particular bond crosses the cutoff value between two optimization steps, the energy derivative (the force) experiences a sudden change. The magnitude of the jump depends on the cutoff value. The default value of 0.001 is normally not a problem during MD but it may break the geometry optimization convergence.

There are two ways to reduce the discontinuity and thus to improve the stability of the geometry optimization. One way is to switch on the 2013 formula for the torsion angles (the tors13=1 key in the control file). This will make the torsion angles change more smoothly at lower bond orders but it will not affect the valence angles. You should be aware, however, that using this option changes the bond order dependence of the ReaxFF 4-center term.

The other way is to decrease the cutof2 value in the control file. This will significantly reduce the discontinuity in the valence angles and somewhat in the torsion angles but will not remove it. This will also make the calculation somewhat slower because more angles will have to be included in the computation.



## WARNINGS

**WARNING: Inconsistent vdWaals-parameters in forcefield. See output** All atom types in a force-field file should normally have consistent Van der Waals screening and short-range repulsion (a.k.a. inner core) parameters. This warning is printed if two atom types have inconsistent parameters.

**WARNING: Suspicious force-field EEM parameters for ...** For every atom type, the eta and gamma parameters for the electronegativity equalization method (EEM) should satisfy the relation:  $\eta > 7.2 \cdot \gamma$ . Otherwise a polarisation catastrophe is likely to occur at a short interatomic distance, the critical distance being dependent on the eta/gamma ratio. The smaller the ratio the larger the distance at which this occurs. When the polarisation catastrophe occurs the amount of charge that flows from one atom to the other can become very large. The EEM routine checks that the resulting charge for each atom lies within the  $[-10, Z]$  interval, where  $Z$  is the number of electrons in the neutral atom, and throws an error if the check fails. The user can override this error by setting the badeem control parameter to 1.



## INCLUDED FORCEFIELDS

See also Included Forcefields (development version)

Description of ReaxFF force fields

Disclaimer: Using these forcefields for systems they have not been explicitly trained against may produce unrealistic results. Please see the full manuscripts for more detailed information.

The force field files used by the SCM version of ReaxFF are compatible with those used by the original ReaxFF code. So if you have the force field information from somewhere else you can just use it (save it in a text file, and select it in ADFinput via the Other... option).

There are currently two major groupings (i.e., the ReaxFF branches) of parameter sets that are intra-transferable with one another: (1) the combustion branch and (2) the aqueous (water) branch. The major difference between these two branches is in the O/H parameters, where the combustion branch focuses on accurately describing water as a gas-phase molecule, and the water branch is targeted at aqueous chemistry.

**AB.ff: (H/O/N/B) Ammonia Borane** M.R.Weismiller, A.C.T. van Duin, J. Lee, R.A. Yetter *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion* *J. Phys. Chem. A* 2010, 114, 5485-5492 (<http://dx.doi.org/10.1021/jp100136c>)

- QM data were generated describing the single and (if relevant) double and triple bond dissociation for all B/N/O/H combinations. These data were used to derive initial ReaxFF bond parameters, and all calculations were performed using DFT with the B3LYP functional and the Pople 6-311G\*\* basis set.
- The training set was then extended with QM data describing angular distortions in a set of small AB-related (AB H<sub>3</sub>N-BH<sub>3</sub>) molecules. These data were used to derive the initial ReaxFF angular parameters.
- The training set was extended with reaction barriers for key reaction steps such as H<sub>2</sub> release from AB, dimerization of H<sub>2</sub>B-NH<sub>2</sub> and reaction energies associated with H<sub>2</sub> release from AB and with AB oxidation.
- Branch: combustion.

**AuCSOH.ff: (Au/C/S/O/H)** J.A. Keith, D. Fantauzzi, T. Jacob, and A.C.T. van Duin *Reactive forcefield for simulating gold surfaces and nanoparticles* *Physical Review B* (2010) 81, 235404-1/235404-8 (<http://dx.doi.org/10.1103/PhysRevB.81.235404>)

- The original Au-Au parameters were extended by three publications:
- Au/O: K. Joshi, A.C.T. van Duin, and T. Jacob Development of a ReaxFF description of gold oxides and initial application to cold welding of partially oxidized gold surfaces *Journal of Materials Chemistry* 20, (2010), 10431-10437 <http://dx.doi.org/10.1039/C0JM01556C>
- Au/C/S/H: T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard Development of interatomic ReaxFF potentials for Au-S-C-H systems *Journal of Physical Chemistry C* 115, (2011), 10315-10322 <http://dx.doi.org/10.1021/jp201496x>

- C/O/H/S: Rahaman, O., van Duin, A. C. T., Goddard, W. A., III, and Doren, D. J. Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization *Journal of Physical Chemistry B* 115 (2011), 249-261 <http://dx.doi.org/10.1021/jp108642r>
- The forcefield does not include Au/N parameters
- Branch: water.

**CHO.ff: (C/H/O) Hydrocarbon oxidation** K.Chenoweth, A.C.T. van Duin, W. A. Goddard *ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation* *J. Phys. Chem. A* 2008, 112, 1040-1053 (<http://dx.doi.org/10.1021/jp709896w>)

- To obtain the H/C/O compound data required to extend the hydrocarbon-training set, DFT calculations were performed on the following systems: (a) dissociation energies for various bonds containing carbon, oxygen, and hydrogen. The ground state structure was obtained through full geometry optimization. Dissociation curves were calculated by constraining only the bond length of interest and re-optimization of the remaining internal coordinates. Optimization was also performed for the various angles and torsions associated with C/H/O interactions.
- Branch: combustion.

**HCONSB.ff: (H/C/O/N/S/B)** M.R. Weismiller, A.C.T. van Duin, J. Lee, and R.A. Yetter, *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion* *J. Phys. Chem. A* (2010), 114, 5485-5492. (<http://dx.doi.org/10.1021/jp100136c>)

- The parameters in this forcefield were extended/improved by two other publications:
- A.M. Kamat, A.C.T. van Duin, and A. Yakovlev *Molecular Dynamics Simulations of Laser-Induced Incandescence of Soot Using an Extended ReaxFF Reactive Force Field*. *Journal of Physical Chemistry A* (2010), 114, 12561-1257 <http://dx.doi.org/10.1021/jp1080302>
- F.Castro-Marcano, A.M. Kamat, M.F. Russo, A.C.T. van Duin, and J.P. Mathews *Combustion of an Illinois No. 6 Coal Char Simulated Using an Atomistic Char Representation and the ReaxFF Reactive Force Field*. *Combustion and Flame* (2012), 159, 23273-1285 <http://dx.doi.org/10.1016/j.combustflame.2011.10.022>
- The C/H/O parameters are the same as in the CHO forcefield, with added S/C, S/H and S/O descriptions. This force field was used in Castro et al, *Combustion and Flame* 2011
- The Boron and Nitrogen parameters are based on (but not identical to) the parameters used in Weismiller et al, *JPC-A* 2010.
- Branch: combustion.

**CuCl-H2O.ff: (Cu/Cl/H/O)** O.Rahaman, A.C.T. van Duin, V.S. Bryantsev, J.E. Mueller, S.D. Solares, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride* *J. Phys. Chem. A* 114 (2010), 3556-3568 (<http://dx.doi.org/10.1021/jp9090415>)

- This forcefield is an extension of: A.C.T. van Duin, V.S. Bryantsev, M.S. Diallo, W.A. Goddard, O. Rahaman, D.J. Doren, D. Raymand, and K. Hermansson *Development and validation of a ReaxFF reactive force field for Cu cation/water interactions and copper metal/metal oxide/metal hydroxide condensed phases* *Journal of Physical Chemistry A* 2010, 114, 9507-9514 <http://dx.doi.org/10.1021/jp102272z>
- Branch: water.

**FeOCHCl.ff: (Fe/O/C/H/Cl)** M.Aryanpour, A.C.T. van Duin, J.D. Kubicki *Development of a Reactive Force Field for Iron-Oxyhydroxide Systems* *J. Phys. Chem. A* 2010, 114, 6298-6307 (<http://dx.doi.org/10.1021/jp101332k>)

- The Cl parameters were published by: O. Rahaman, A.C.T. van Duin, V.S. Bryantsev, J.E. Mueller, S.D. Solares, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride* *J. Phys. Chem. A* 114 (2010), 3556-3568 <http://dx.doi.org/10.1021/jp9090415>

- The initial force field parameters for the Fe-Fe parameters were taken from an earlier force field development project on bulk-iron metal, based on DFT-calculations on antiferromagnetic BCC and FCC. The ReaxFF parameters have not been published yet, however the DFT data can be found in ref 31 of the above mentioned manuscript. The O/H parameters were taken from the ReaxFF bulk water description. The Fe/Fe and O/H parameters were kept fixed to these initial values, whereas the Fe/O parameters were reoptimized against the quantum mechanical results presented in the above mentioned manuscript.
- Detailed information on the force field parameters is given in the supporting information of the above mentioned manuscript.
- Branch: water.

**HE.ff: (C/H/O/N) RDX/High Energy** L.Z. Zhang, A.C.T. van Duin, S.V. Zybin, and W.A. Goddard *Thermal Decomposition of Hydrazines from Reactive Dynamics Using the ReaxFF Reactive Force Field* *Journal of Physical Chemistry B* (2009) 113, 10770-10778 (<http://dx.doi.org/10.1021/jp900194d>)

- Part of this forcefield is also published in: L.Z. Zhang, S.V. Zybin, A.C.T. van Duin, S. Dasgupta, W.A. Goddard, and E.M. Kober Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations *Journal of Physical Chemistry A* (2009) 113, 10619-10640 <http://dx.doi.org/10.1021/jp901353a>
- The parameters of the nitramine ReaxFF are based on a large number of ab initio QM calculations. Over 40 reactions and over 1600 equilibrated molecules have been used; they are designed to characterize the atomic interactions under various environments likely and unlikely high energy each atom can encounter. The training set contains bond breaking and compression curves for all possible bonds, angle and torsion bending data for all possible cases, as well as crystal data.
- Please see the supplemental material from Phys. Rev. Lett. 2003, 91, 098301 for a detailed description of the parameterization of this force field.
- Branch: combustion.

**NaH.ff: (Na/H)** J.G.O. Ojwang, R. Van Santen, G.J. Kramer, A.C.T van Duin, and W.A Goddard *Modeling the sorption dynamics of NaH using a reactive force field* *Journal of Chemical Physics* 2008, 128, 164714 (<http://dx.doi.org/10.1063/1.2908737>)

- This forcefield originally had a typo, defining the H-Na-Na angle twice. The same typo is in table 4 of the publication, but the text clearly mentions that the second line should define Na-H-Na instead.
- Branch: combustion.

**NiCH.ff: (Ni/C/H)** J.E. Mueller, A.C.T. van Duin, and W.A. Goddard III *Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel* *J. Phys. Chem. C* 2010, 114, 4939-4949 (<http://dx.doi.org/10.1021/jp9035056>)

- Branch: combustion.

**SiOH.ff: (Si/O/H)** J.C. Fogarty, H.M. Aktulga, A.Y. Grama, A.C.T. van Duin, S.A. Pandit *A reactive molecular dynamics simulation of the silica-water interface* *J. Chem. Phys.* 2010, 132, 174704 (<http://dx.doi.org/10.1063/1.3407433>)

- This force field was trained to model the interaction of water at the SiO<sub>2</sub> surface, with specific emphasis on proton-transfer reactions. Updated parameters were fitted for all Si/O/H bond, angle, and torsion interactions as well, in addition to the dissociation of a water molecule from a single Si(OH)<sub>4</sub> molecule and reaction energies for the polymerization of Si(OH)<sub>4</sub>
- Branch: water.

**SiC.ff: (Si/C/O/H/N/S)** D.Newsome, D. Sengupta, H. Foroutan, M.F. Russo, and A.C.T. van Duin *Oxidation of Silicon Carbide by O<sub>2</sub> and H<sub>2</sub>O: A ReaxFF Reactive Molecular Dynamics Study, Part I* *Journal of Physical Chemistry* 2012 116, 16111-16121 (<http://dx.doi.org/10.1021/jp306391p>)

- The included forcefield is based on the Newsome reference, with slightly improved parameters by van Duin et al.
- Branch: combustion.

**VOCH.ff: (V/O/C/H)** K.Chenoweth, A.C.T. van Duin, P. Persson, M.J. Cheng, J. Oxgaard, W.A. Goddard *Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts* *J. Phys. Chem. C*, 2008, 112, 14645-14654 (<http://dx.doi.org/10.1021/jp802134x>)

- The ReaxFF force field parameters have been fit to a large quantum mechanics (QM) training set containing over 700 structures and energetics related to bond dissociations, angle and dihedral distortions, and reactions between hydrocarbons and vanadium oxide clusters. In addition, the training set contains charge distributions for small vanadium oxide clusters and the stabilities of condensed-phase systems including V<sub>2</sub>O<sub>5</sub>, VO<sub>2</sub>, and V<sub>2</sub>O<sub>3</sub> in addition to metallic V (V<sub>0</sub>).
- Branch: combustion.

**ZnOH.ff: (Zn/O/H)** D.Raymand, A.C.T. van Duin, M. Baudin, K. Hermansson *A reactive force field (ReaxFF) for zinc oxide* *Surface Science* 2008, 602, 1020-1031 (<http://dx.doi.org/10.1016/j.susc.2007.12.023>)

- updated version published by: D. Raymand, A.C.T. van Duin, D. Spangberg, W.A. Goddard, K. Hermansson *Water adsorption on stepped ZnO surfaces from MD simulation* *Surface Science* 2010, 604, 9-10, 741-752 <http://dx.doi.org/10.1016/j.susc.2009.12.012>
- Based on QM calculations for Zn(s), ZnO(s), and Zn hydroxide clusters [Zn(OH)<sub>2</sub> and O(ZnOH)<sub>2</sub>], ReaxFF parameters were generated for Zn-O and Zn-Zn bond energies and for Zn-O-Zn, O-Zn-O, O-Zn-Zn and Zn-O-H valence angle energies.
- QM calculations were performed for the four crystal polymorphs of the wurtzite, zincblende, rocksalt and caesium chloride structures (the structures are also referred to as h-ZnS, c-ZnS, NaCl and CsCl, respectively).
- Branch: water.

**Al-H<sub>2</sub>O.ff: (Al/H/O)** M.Russo, R. Li, M. Mench, and A.C.T. van Duin *Molecular Dynamic Simulation of Aluminum-Water Reactions Using the ReaxFF Reactive Force Field* *International Journal of Hydrogen Energy* 36 (2011), 5828-5835 (<http://dx.doi.org/10.1016/j.ijhydene.2011.02.035>)

- Branch: water.

**CaSiAlO.ff: (C/H/O/Fe/Cl/Si/Al/Ca)** M.C. Pitman and A.C.T. van Duin *Dynamics of Confined Reactive Water in Smectite Clay-Zeolite Composites* *J. Am. Chem. Soc.*, 2012, 134 (6), 3042-3053 (<http://dx.doi.org/10.1021/ja208894m>)

- Branch: water.

**dispersion/CHONSSi-Ig.ff: (C/H/O/N/S/Si)** L.Liu, Y. Liu, S.V. Zybin, H. Sun, and W.A. Goddard III *ReaxFF-Ig: Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials* *The Journal of Physical Chemistry A*, 2011, 115(40), 11016-11022 (<http://dx.doi.org/10.1021/jp201599t>)

- This forcefield adds London dispersion correction terms to reaxFF, and is optimized for the energetic materials RDX, PETN, TATB, and NM plus graphite, polyethylene, solid carbon dioxide, and solid N<sub>2</sub>, using the low temperature crystal structures to determine the Ig correction parameters.
- Branch: combustion.

**CHOFeAlNiCuS.ff: (C/H/O/Fe/Al/Ni/Cu/S)** O.Rahaman, A.C.T. van Duin, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization* *Journal of Physical Chemistry B* 115 (2011), 249-261. (<http://dx.doi.org/10.1021/jp204894m>)

- C/O/H parameters only. The Cu/Fe/Al/Ni parameters are from: Y.K. Shin, H. Kwak, C. Zou, A.V. Vasenkov, and A.C.T. van Duin *Development and Validation of a ReaxFF Reactive Force Field for*



Fe/Al/Ni Alloys: Molecular Dynamics Study of Elastic Constants, Diffusion, and Segregation *J. Phys. Chem. A*, 2012, 116 (49), pp 12163–12174 <http://dx.doi.org/10.1021/jp308507x>

- Not all cross-terms between the two forcefield files are defined, which might cause problems if the system has (for example) C-Cu interactions.

- Branch: water.

**AuSCH\_2011.ff: (Au/S/C/H)** T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard III, *Development of Interatomic ReaxFF Potentials for Au-S-C-H Systems* *J. Phys. Chem. A*, 115, 10315-10322 (2011) (<http://dx.doi.org/10.1021/jp201496x>)

- Branch: combustion.

**AuSCH\_2013.ff: (Au/S/C/H)** Gyun-Tack Bae and Christine M. Aikens *Improved ReaxFF Force Field Parameters for Au-S-C-H Systems* *Journal of Physical Chemistry A* 2013 117 (40), 10438-10446 (<http://dx.doi.org/10.1021/jp405992m>)

- Based upon: T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard Development of interatomic ReaxFF potentials for Au-S-C-H systems. *Journal of Physical Chemistry C* 115, (2011), 10315-10322.
- yields improvements for bond bending potential energy surfaces
- aims to agree with DFT geometries of small clusters and gold-thiolate nanoparticles
- Branch: combustion.

**PDMSDecomp.ff: (C/H/O/Si)** K.Chenoweth, S. Cheung, A.C.T. van Duin, W.A. Goddard III, and E.M. Kober *Simulations on the Thermal Decomposition of a Poly(dimethylsiloxane) Polymer Using the ReaxFF Reactive Force Field* *J. Am. Chem. Soc.*, 2005, 127 (19), pp 7192-7202 (<http://dx.doi.org/10.1021/ja050980t>)

- Specialized forcefield, designed to “investigate the failure of the poly(dimethylsiloxane) polymer (PDMS) at high temperatures and pressures and in the presence of various additives”
- Line from the torsion block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: combustion.

**TiOCHNCl.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F)** S.Y. Kim, A.C.T. van Duin, and J.D. Kubicki *Molecular dynamics simulations of the interactions between TiO<sub>2</sub> nanoparticles and water with Na<sup>+</sup> and Cl<sup>-</sup>, methanol, and formic acid using a reactive force field* *Journal of Materials Research / Volume 28 / Issue 03 / 2013*, pp 513-520 (<http://dx.doi.org/10.1557/jmr.2012.367>)

- used for simulating TiO<sub>2</sub>(both rutile and anatase) nanoparticles with water, methanol, and formic acid
- The force field was validated by comparing water dissociative adsorption percentage and bond length between Na-O with density functional theory (DFT) and experimental results
- Branch: water.

**PtCH.ff: (C/H/Pt)** C.F. Sanz-Navarro, P. Astrand, De Chen, M. Ronning, A.C.T. van Duin, T. Jacob, and W.A. Goddard III *Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets* *J. Phys. Chem. A* 112, 1392-1402 (2008) (<http://dx.doi.org/10.1021/jp074806y>)

- Branch: combustion.

**BaYZrCHO.ff: (C/H/O/Ba/Zr/Y)** A.C.T. van Duin, B.V. Merinov, S.S. Jang, and W.A. Goddard III *ReaxFF Reactive Force Field for Solid Oxide Fuel Cell Systems with Application to Oxygen Ion Transport in Yttria-Stabilized Zirconia* *J. Phys. Chem. A*, 112, 3133-3140 (2008) (<http://dx.doi.org/10.1021/jp076775c>)

- Branch: combustion.

**CHONSSiPtZrNiCuCo.ff: (C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co)** K.D. Nielson, A.C.T. van Duin, J. Oxgaard, W.Q. Deng, and W.A. Goddard III *Development of the ReaxFF Reactive Force Field for Describing Transition Metal*

*Catalyzed Reactions, with Application to the Initial Stages of the Catalytic Formation of Carbon Nanotubes* J. Phys. Chem. A, 109, 493-499 (2005) (<http://dx.doi.org/10.1021/jp046244d>)

- Branch: combustion.

**Glycine.ff: (C/H/O/N)** O.Rahaman, A.C.T. van Duin, W.A. Goddard III, and D.J. Doren, *Development of a ReaxFF Reactive Force Field for Glycine and Application to Solvent Effect and Tautomerization* J. Phys. Chem. B, 115, 249-261 (2011) (<http://dx.doi.org/10.1021/jp108642r>)

- Line from the valence angle block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: water.

**SiONH.ff: (C/H/O/N/Si/S)** A.D. Kulkarni, D.G. Truhlar, S.G. Srinivasan, A.C.T. van Duin, P. Norman, and T.E. Schwartzentruber *Oxygen Interactions with Silica Surfaces: Coupled Cluster and Density Functional Investigation and the Development of a New ReaxFF Potential* J. Phys. Chem. C, 2013, 117 (1), pp 258-269 (<http://dx.doi.org/10.1021/jp3086649>)

- Aimed at oxygen interactions with realistic silica surfaces
- Lines from the valence angle block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: combustion.

**CHOFe.ff: (C/H/O/Fe/Ci/Si/Al)** Chenyu Zou, A.C.T. Van Duin *Investigation of Complex Iron Surface Catalytic Chemistry Using the ReaxFF Reactive Force Field Method* JOM, December 2012, Volume 64, Issue 12, pp 1426-1437 (<http://dx.doi.org/10.1007/s11837-012-0463-5>)

- only the parameters for Fe (and crossterms) differ from the CHOAlSi.ff forcefield
- Branch: water.

**CHOAlSi.ff: (C/H/O/Fe/Ci/Si/Al)** F.Castro-Marcanao, A.C.T. van Duin *Comparison of thermal and catalytic cracking of 1-heptene from ReaxFF reactive molecular dynamics simulations* Combustion and Flame, Volume 160, Issue 4, April 2013, Pages 766-775 (<http://dx.doi.org/10.1016/j.combustflame.2012.12.007>)

- only the parameters for Fe (and crossterms) differ from the CHOFe.ff forcefield
- Branch: water.

**CHOLi.ff: (C/H/O/N/S/Mg/P/Na/Li)** D.Bedrov, G.D. Smith, A.C.T. van Duin *Reactions of Singly-Reduced Ethylene Carbonate in Lithium Battery Electrolytes: A Molecular Dynamics Simulation Study Using the ReaxFF* Journal of Physical Chemistry A, 2012, 116 (11), pp 2978-2985 (<http://dx.doi.org/10.1021/jp210345b>)

- specifically generated for simulating Lithium battery electrolytes
- must be used in combination with the MOLCHARGE keyword to set a charge restraint on Li and CO<sub>3</sub>!
- Branch: water.

**SiOAlLi.ff: (H/O/Si/Al/Li)** B.Narayanan, A.C.T. van Duin, B.B. Kappes, I.E. Reimanis and C.V. Ciobanu *A reactive force field for lithium-aluminum silicates with applications to eucryptite phases* Modelling and Simulation in Materials Science and Engineering 2012 20 015002 (<http://dx.doi.org/10.1088/0965-0393/20/1/015002>)

- Branch: water.

**PdO.ff: (Pd/O)** T.P. Senftle, R.J. Meyer, M.J. Janik and A.C.T. van Duin *Development of a ReaxFF potential for Pd/O and application to palladium oxide formation* The Journal of Chemical Physics 139, 044109 (2013) (<http://dx.doi.org/10.1063/1.4815820>)

- used for studying Oxidation states of Pd nanoparticles, surfaces and bulk configurations with a GCMC method

- Branch: combustion.

**PdH.ff: (Pd/H)** T.P. Senftle, M.J. Janik and A.C.T. van Duin *A ReaxFF Investigation of Hydride Formation in Palladium Nanoclusters via Monte Carlo and Molecular Dynamics Simulations* *The Journal of Physical Chemistry C*, 2014, 118 (9), pp 4967-4981 (<http://dx.doi.org/10.1021/jp411015a>)

- used in combination with a GCMC method
- Branch: combustion.

**Co.ff: (Co)** Xue-Qing Zhang, E. Iype, S.V. Nedeia, A.P.J. Jansen, B.M. Szyja, E.J.M. Hensen, and R.A. van Santen *Site Stability on Cobalt Nanoparticles: A Molecular Dynamics ReaxFF Reactive Force Field Study* *The Journal of Physical Chemistry C*, 2014, 118 (13), pp 6882-6886 (<http://dx.doi.org/10.1021/jp500053u>)

- forcefield was generated using a recently developed Monte Carlo algorithm with simulated annealing.
- Branch: combustion.

**CHONSMgPNaCuCl.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl)** Susanna Monti, Cui Li, and Vincenzo Carravetta *Reactive Dynamics Simulation of Monolayer and Multilayer Adsorption of Glycine on Cu(110)* *J. Phys. Chem. C*, 2013, 117 (10), pp 5221-5228 (<http://dx.doi.org/10.1021/jp312828d>)

- Reactive MD-force field for amino acids on copper
- Branch: water.

**CHOSMoNiLiBFPN.ff: (C/H/O/S/Mo/Ni/Li/B/F/P/N)** Md M. Islam, V.S. Bryantsev, A.C.T. van Duin *ReaxFF Reactive Force Field Simulations on the Influence of Teflon on Electrolyte Decomposition during Li/SWCNT Anode Discharge in Lithium-Sulfur Batteries* *J. Electrochem. Soc.* 2014 volume 161, issue 8, E3009-E3014 (<http://dx.doi.org/10.1149/2.005408jes>)

- forcefield for Electrochemistry in Li-S batteries
- Branch: combustion.

**CHONSSiNaFZr.ff: (C/H/O/N/S/Si/Na/F/Zr)** A.Rahnamoun and A.C.T. van Duin *Reactive Molecular Dynamics Simulation on the Disintegration of Kapton, POSS Polyimide, Amorphous Silica, and Teflon during Atomic Oxygen Impact Using the Reaxff Reactive Force-Field Method* *J. Phys. Chem. A*, 2014, 118 (15), pp 2780-2787 (<http://dx.doi.org/10.1021/jp4121029>)

- comments in the forcefield file: interactions with water and Na+ Fogarty et al. JCP-2010 ; with glycine + C/H/F parameters; Si-F bond/offdiag/angle parameters; Si-S dummy parameters + S-O-H parameters(Yun 2012 Oct8) + H-F bond/offdiag (Jan14 2013 Joon) Jan31: added Zr/O/H/C
- Branch: water.

**TiClOH.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F)** Sung-Yup Kim and A.C.T. van Duin *Simulation of Titanium Metal/Titanium Dioxide Etching with Chlorine and Hydrogen Chloride Gases Using the ReaxFF Reactive Force Field* *J. Phys. Chem. A*, 2013, 117 (27), pp 5655-5663 (<http://dx.doi.org/10.1021/jp4031943>)

- adaptation/evolution of the TiOCHNCl.ff forcefield by Kim, S.-Y. et al.
- Branch: water.

**CHONSSiNaAl.ff: (C/H/O/N/S/Si/Na/Al)** C.Bai, L. Liu, and H. Sun *Molecular Dynamics Simulations of Methanol to Olefin Reactions in HZSM-5 Zeolite Using a ReaxFF Force Field* *J. Phys. Chem. C*, 2012, 116 (12), pp 7029-7039 (<http://dx.doi.org/10.1021/jp300221j>)

- used to simulate methanol to olefin (MTO) reactions in H-ZSM-5 zeolite
- Branch: water.

**undocumented/NiCH.ff: (Ni/C/H/O/N/S/F/Pt/Cl)** Unknown *No Name* Not published (<http://>)

- This forcefield is from april 2009, and is not published

- Branch: combustion.

**LiS.ff: (Li/S)** Md M. Islam, A. Ostadhossein, O. Borodin, A.T. Yeates, W.W. Tipton, R.G. Hennig, N. Kumar, and A.C.T. van Duin *ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials Phys. Chem. Chem. Phys.*, 2015,17, 3383-3393 (<http://dx.doi.org/10.1039/C4CP04532G>)

- Developed for and used to study Sulfur cathode behaviour in Li battery cells
- Branch: combustion.

**CHONSSiPtNiCuCoZrYBa.ff: (C/H/O/N/S/Si/Pt/Ni/Cu/Co/Zr/Y/Ba)** B.V. Merinov, J.E. Mueller, A.C.T. van Duin, Qi An, and W.A. Goddard III *ReaxFF Reactive Force-Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell J. Phys. Chem. Lett.*, 2014, 5 (22), pp 4039-4043 (<http://dx.doi.org/10.1021/jz501891y>)

- Force field was developed by combining the YSZ and Ni/C/H descriptions
- From the summary: “The products obtained in our simulations are the same as those in experiment, which indicates that the developed ReaxFF potential properly describes complex physicochemical processes, such as the oxide-ion diffusion, fuel conversion, water formation reaction, coking, and delamination, occurring at the TPB and can be recommended for further computational studies of the fuel/electrode/electrolyte interfaces in a SOFC”
- The Aa atom type is a rename of the Zr atom type, which was defined twice.
- Branch: combustion.

**CHONSSiNaP.ff: (C/H/O/N/S/Si/Na/P)** Bo Zhang, A.C.T. van Duin and J.K. Johnson *Development of a ReaxFF Reactive Force Field for Tetrabutylphosphonium Glycinate/CO2 Mixtures J. Phys. Chem. B*, 2014, 118 (41), pp 12008-12016 (<http://dx.doi.org/10.1021/jp5054277>)

- The forcefield file mentions “Gly with dummy N-P parameters”
- It was developed for studying Carbon dioxide interactions with the ionic liquid tetrabutylphosphonium glycinate, both physical and chemical absorption.
- Several lines from valence angle block were referring to non-existent atoms from the atomic block and thus were removed.
- Branch: combustion.

**CHOLi\_2.ff: (C/H/O/Li)** M.Raju, P. Ganesh, P.R.C. Kent, and A.C.T. van Duin *Reactive Force Field Study of Li/C Systems for Electrical Energy Storage J. Chem. Theory Comput.*, 2015, 11 (5), pp 2156-2166 (<http://dx.doi.org/10.1021/ct501027v>)

- Used for studying Li/C systems with GCMC and MD
- Also contains parameters for “Vi” and “GI”, but these virtual elements are not mentioned in the paper
- Parameters were fitted using a training set consisting, amongst others, of Li binding energies on pristine graphene and graphite, Li migration pathways in graphite and Li dissociation pathways in different hydrocarbons
- The forcefield was validated by a side-by-side comparison of ReaxFF and DFT energies for Li binding on a divacancy, and ReaxFF and DFT ground-state configurations for stage II and stage I stacking in graphite obtained using GCMC simulations
- The forcefield reproduces the in-plane Li ordering as well as the graphite stacking sequence for stage II and stage I compounds
- Branch: water.

**CHONSSiCaCsKsSrNaMgAlCu.ff: (C/H/O/N/S/Si/Ca/Cs/K/Sr/Na/Mg/Al/Cu)** G.M. Psfogiannakis, J.F. McCleerey, E. Jaramillo and A.C.T. van Duin *ReaxFF Reactive Molecular Dynamics Simulation of the Hydra-*

*tion of Cu-SSZ-13 Zeolite and the Formation of Cu Dimers* J. Phys. Chem. C, 2015, 119 (12), pp 6678-6686 (<http://dx.doi.org/10.1021/acs.jpcc.5b00699>)

- This Cu/Si/Al/O/H forcefield was developed for and used in MD simulations of the hydration of Cu-exchanged SSZ-13 catalyst.
- The force field was developed by merging and expanding previously tested and published ReaxFF force fields for Si/Al/O/H systems and Cu/O/H systems (citations 19-26 of the publication)
- This forcefield is an extension of K.L. Joshi et al 2014, <http://dx.doi.org/10.1039/C4CP02612H>, all non-Cu parameters are the same.
- Branch: water.

**HOSMg.ff: (H/O/S/Mg)** E.Iype, M. Hütter, A.P.J. Jansen, S.V. Nedea and C.C.M. Rindt *Parameterization of a reactive force field using a Monte Carlo algorithm* J. Comput. Chem., 2013, 34: 1143-1154 (<http://dx.doi.org/10.1002/jcc.23246>)

- This forcefield is optimized with a metropolis Monte-Carlo algorithm with simulated annealing to search for the optimum parameters for the ReaxFF force field in a high-dimensional parameter space.
- The optimization is done against a set of quantum chemical data for MgSO<sub>4</sub> hydrates.
- Branch: combustion.

**CHONSMgPNaCuCl\_v2.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl)** S.Monti, A. Corozzi, P. Fristrup, K.L. Joshi, Yun Kyung Shin, P. Oelschlaeger, A.C.T. van Duin and V. Baronee *Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field* Phys. Chem. Chem. Phys., 2013, 15, 15062-15077 (<http://dx.doi.org/10.1039/C3CP51931G>)

- This forcefield is an extension of CHONSMgPNaCuCl.ff by S. Monti et al., J. Phys. Chem. C, 2013, 117 (10), pp 5221-5228, <http://dx.doi.org/10.1021/jp312828d>
- Developed for peptide and protein simulations
- Branch: water.

**OPt.ff: (O/Pt)** D.Fantauzzi, J. Bandlow, L. Sabo, J.E. Mueller, A.C.T. van Duin and T. Jacob *Development of a ReaxFF potential for Pt-O systems describing the energetics and dynamics of Pt-oxide formation* Phys. Chem. Chem. Phys., 2014, 16, 23118-23133 (<http://dx.doi.org/10.1039/C4CP03111C>)

- Pt-Pt parameters for bulk platinum phases, low & high-index platinum surfaces and nanoclusters.
- O-Pt parameters for bulk platinum oxides, as well as oxygen adsorption and oxide formation on Pt(111) terraces and the {111} and {100} steps connecting them.
- Branch: combustion.

**CHONSMgPNaTiClF.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F)** Stijn Huygh, Annemie Bogaerts, Adri C.T. van Duin and Erik C. Neyts *Development of a ReaxFF reactive force field for intrinsic point defects in titanium dioxide* Computational Materials Science, Volume 95, December 2014, Pages 579-591, ISSN 0927-0256 (<http://dx.doi.org/10.1016/j.commatsci.2014.07.056>)

- Forcefield developed for studying the influence of intrinsic point defects on the chemistry with TiO<sub>2</sub> condensed phases.
- Forcefield seems to be based on TiOCHNCl.ff, <http://dx.doi.org/10.1557/jmr.2012.367>
- Branch: water.

**LiSi.ff: (Li/Si)** A.Ostadossein, E.D. Cubuk, G.A. Tritsarlis, E. Kaxiras, S. Zhanga and A.C.T. van Duin *Stress effects on the initial lithiation of crystalline silicon nanowires: reactive molecular dynamics simulations using ReaxFF* Phys. Chem. Chem. Phys., 2015, 17, 3832-3840 (<http://dx.doi.org/10.1039/C4CP05198J>)

- Branch: combustion.

**CHOFeAlNiCuSCr.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr)** Y.K. Shin, H. Kwak, A.V. Vasenkov, D. Sengupta and A.C.T. van Duin *Development of a ReaxFF Reactive Force Field for Fe/Cr/O/S and Application to Oxidation of Butane over a Pyrite-Covered Cr<sub>2</sub>O<sub>3</sub> Catalyst* ACS Catalysis, 2015, 5 (12), pp 7226-7236 (<http://dx.doi.org/10.1021/acscatal.5b01766>)

- Forcefield optimized for Fe/Cr/O/S
- Branch: water.

**CHOFeAlNiCuSCr\_v2.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr) Ni-O-vacancy** C.Zou et al. *Molecular dynamics simulations of the effects of vacancies on nickel self-diffusion, oxygen diffusion and oxidation initiation in nickel, using the ReaxFF reactive force field* Acta Materialia, Volume 83, 15 January 2015, Pages 102-112 (<http://dx.doi.org/10.1016/j.actamat.2014.09.047>)

- Forcefield optimized for Ni/O, trained with a QM data on Ni, NiO and vacancies
- The non-carbon parameters are the same as in CHOFeAlNiCuSCr\_v3.ff
- Branch: water.

**CHOFeAlNiCuSCr\_v3.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr)** F.Tavazza, T.P. Senftle, C. Zou, C.A. Becker and A.C.T van Duin *Molecular Dynamics Investigation of the Effects of Tip-Substrate Interactions during Nanoindentation* J. Phys. Chem. C, 2015, 119 (24), pp 13580-13589 (<http://dx.doi.org/10.1021/acs.jpcc.5b01275>)

- Combination of the C.ff (condensed carbon) forcefield with Ni/C/O/H parameters
- The non-carbon parameters are the same as in CHOFeAlNiCuSCr\_v2.ff
- Branch: water.

**C.ff: (C) C-2013** S.G. Srinivasan, A.C.T. van Duin and P. Ganesh *Development of a ReaxFF Potential for Carbon Condensed Phases and Its Application to the Thermal Fragmentation of a Large Fullerene* J. Phys. Chem. A, 2015, 119 (4), pp 571-580 (<http://dx.doi.org/10.1021/jp510274e>)

- Forcefield designed for modeling Carbon condensed phases
- Branch: combustion.

**CHONSSiGe.ff: (C/H/O/N/S/Si/Ge)** G.Psofogiannakis and A.C.T van Duin *Development of a ReaxFF reactive force field for Si/Ge/H systems and application to atomic hydrogen bombardment of Si, Ge, and SiGe (100) surfaces* Surface Science 2016, Vol. 646, pp 253-260 (<http://dx.doi.org/10.1016/j.susc.2015.08.019>)

- Forcefield designed for bombardment of Si, Ge and SiGe surfaces with atomic hydrogen.
- Branch: combustion.

**CHONSPtCINi.ff: (C/H/O/N/S/F/Pt/Cl/Ni) Water-Pt-Ni-Nafion** D.Fantauzzi, J.E. Mueller, L. Sabo, A.C.T. van Duin and T. Jacob *Surface Buckling and Subsurface Oxygen: Atomistic Insights into the Surface Oxidation of Pt(111)* ChemPhysChem, 2015, Vol.16: 2797-2802 (<http://dx.doi.org/10.1002/cphc.201500527>)

- extension of the OPt.ff forcefield parameters
- Branch: water.

**CHONSSiPtZrNiCuCoHeNeArKrXe.ff: (C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co/He/Ne/Ar/Kr/Xe)** A.M. Kamat, A.C.T. van Duin and A. Yakovlev *Molecular Dynamics Simulations of Laser-Induced Incandescence of Soot Using an Extended ReaxFF Reactive Force Field* J. Phys. Chem. A, 2010, 114 (48), pp 12561-12572 (<http://dx.doi.org/10.1021/jp1080302>)

- forcefield designed for the study of Laser-induced incandescence of soot
- Branch: combustion.



**CHOSFCIN.ff: (C/H/O/S/F/Cl/N)** M.A. Wood, A.C.T. van Duin and A. Strachan *Coupled Thermal and Electromagnetic Induced Decomposition in the Molecular Explosive alpha-HMX; A Reactive Molecular Dynamics Study* J. Phys. Chem. A, 2014, 118 (5), pp 885-895 (<http://dx.doi.org/10.1021/jp406248m>)

- forcefield designed for studying the combustion of the high-energy material a-HMX
- Branch: combustion.

**Mue2016.ff: (C/H/O/S)** Julian Mueller and Bernd Hartke *ReaxFF Reactive Force Field for Disulfide Mechanochemistry, Fitted to Multireference ab Initio Data;* J. Chem. Theory Comput., 2016, xxx, xxx (<http://dx.doi.org/10.1021/acs.jctc.6b00461>)

- forcefield for studying S-S bond ruptures in mechanophores upon mechanical stress. Ambient conditions, both in gas phase and toluene solvent.
- Branch: combustion.

**CBN.ff: (C/H/B/N)** Sung Jin Pai, Byung Chul Yea and Sang Soo Han *Reactive force field for the improved design of liquid CBN hydrogen storage materials* Phys. Chem. Chem. Phys., 2016, 18, pp 1818-1827 (<http://dx.doi.org/10.1039/C5CP05486A>)

- forcefield for studying liquid CBN (carbon-boron-nitrogen) hydrogen-storage materials.
- Branch: combustion.

**AgZnO.ff: (C/H/O/N/Si/Cu/Ag/Zn)** A.Lloyd, D. Cornil, A.C.T. van Duin, D. van Duin, R. Smith, S.D. Kenny, J. Cornil and D. Beljonne *Development of a ReaxFF potential for Ag/Zn/O and application to Ag deposition on ZnO* Surface Science, 2016, 645, pp 67-73 (<http://dx.doi.org/10.1016/j.susc.2015.11.009>)

- ReaxFF potential for Ag/Zn/O used to study Ag deposition on ZnO.
- Branch: water.

**AlCHO.ff: (Al/C/H/O)** Sungwook Hong and Adri C. T. van Duin *Atomistic-Scale Analysis of Carbon Coating and Its Effect on the Oxidation of Aluminum Nanoparticles by ReaxFF-Molecular Dynamics Simulations* J. Phys. Chem. C, 2016, 120 (17), pp 9464-9474 (<http://dx.doi.org/10.1021/acs.jpcc.6b00786>)

- ReaxFF potential for Al/C interactions. Used to investigate carbon coating and its effect on the oxidation of aluminum nanoparticles (ANPs)
- Branch: water.

**CHNa.ff: (C/H/Na)** E.Hjertenaes, A.Q. Nguyen and H. Koch *A ReaxFF force field for sodium intrusion in graphitic cathodes* Phys. Chem. Chem. Phys., 2016, 18, pp 31431-31440 (<http://dx.doi.org/10.1039/C6CP06774C>)

- The force field is applied in hybrid grand canonical Monte Carlo-molecular dynamics (GC-MC/MD) simulations of model systems representative of sodium intrusion in graphitic carbon cathodes used in aluminium electrolysis.
- Branch: combustion.

**CuBTC.ff: (C/H/O/N/S/Mg/P/Na/Cu)** L.Huang, T. Bandosz, K. L. Joshi, A. C. T. van Duin and K. E. Gubbins *Reactive adsorption of ammonia and ammonia/water on CuBTC metal-organic framework: A ReaxFF molecular dynamics simulation* J. Chem. Phys., 2013, 138, 034102 (<http://dx.doi.org/10.1063/1.4774332>)

- The force field was used to study reactive adsorption of NH<sub>3</sub> on the dehydrated CuBTC metal-organic framework.
- Branch: water.

**CHONSMgPNaTiClFAu.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F/Au)** Susanna Monti, Vincenzo Carravetta, and Hans Ågren *Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics* J. Phys. Chem. Lett., 2016, 7 (2), pp 272-276 (<http://dx.doi.org/10.1021/acs.jpcclett.5b02769>)

- The force field was designed to study gold-protein interactions in water.

**HOSiAILi.ff: (H/O/Si/Al/Li)** Alireza Ostadhossein, Sung-Yup Kim, Ekin D. Cubuk, Yue Qi, and Adri C. T. van Duin *Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> Electrodes of Lithium Ion Batteries: ReaxFF Reactive Force Field Modeling* *J. Phys. Chem. A*, 2016, 120 (13), pp 2114-2127 (<http://dx.doi.org/10.1021/acs.jpca.5b11908>)

- Developed for studying the energetics and kinetics of lithiation, as well as Li transportation within the crystalline/amorphous silica and alumina phases.

**CHArHeNeKr.ff: (C/H/Ar/He/Ne/Kr)** Kichul Yoon, A. Rahnamoun, J.L. Swett, V. Iberi, D.A. Cullen, I.V. Vlas-siouk, A. Belianinov, S. Jesse, X. Sang, O.S. Ovchinnikova, A.J. Rondinone, R.R. Unocic, and A.C.T. van Duin *Atomistic-Scale Simulations of Defect Formation in Graphene under Noble Gas Ion Irradiation* *ACS Nano*, 2016, 10 (9), pp 8376-8384 (<http://dx.doi.org/10.1021/acs.nano.6b03036>)

- Developed for studying noble gas ion irradiation of graphene and the subsequent effects of annealing. Lattice defects including nanopores were generated.

**CHO-radiation.ff: (C/H/O)** Roger Smith, K. Jolley, C. Latham, M. Heggie, A van Duin, D. van Duin, Houzheng Wu *A ReaxFF carbon potential for radiation damage studies* *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, Volume 393, 15 February 2017, Pages 49-53, (<http://dx.doi.org/10.1016/j.nimb.2016.11.007>)

- Developed forcefield reproduces the formation energies of many of the defects predicted by the ab initio calculations of energetic impacts and collision cascades in graphite.
- Forcefield reproduces the formation energies of many of the defects predicted by the ab initio calculations and the energy pathways between different defect states, which are important for investigating long term defect evolution.

**HOTiPd.ff: (H/O/Ti/Pd)** Rafik Addou, T.P. Senftle, N. O'Connor, M.J. Janik, A.C.T. van Duin, and M. Batzill *Influence of Hydroxyls on Pd Atom Mobility and Clustering on Rutile TiO<sub>2</sub>(011)-2 x 1* *ACS Nano*, 2014, 8 (6), pp 6321-6333 (<http://dx.doi.org/10.1021/nn501817w>)

- Developed for MC simulations of Pd on TiO<sub>2</sub> surfaces.

**CHONSMgPNaFBLi-e.ff: (C/H/O/N/S/Mg/P/Na/F/B/Li)** M.Islam and A.C.T van Duin *Reductive Decomposition Reactions of Ethylene Carbonate by Explicit Electron Transfer from Lithium: An eReaxFF Molecular Dynamics Study* *J. Phys. Chem. C*, 2016, 120 (48), pp 27128-27134 (<http://dx.doi.org/10.1021/acs.jpcc.6b08688>)

- This forcefield uses the ACKS2 charge model
- This forcefield is an eReaxFF forcefield
- Developed for the study of lithium-ion batteries

**CHOFeAlNiCuSCrSiGe.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr/Si/Ge)** Y.Zheng, S. Hong, G. Psfogiannakis, S. Datta, B. Rayner, A.C.T. van Duin and R. Engel-Herbert *Modeling and In-situ Probing of Surface Reactions in Atomic Layer Deposition* *ACS Appl. Mater. Interfaces*, 2017, 9 (18), pp 15848-15856 (<http://dx.doi.org/10.1021/acsami.7b01618>)

- Used for studying the ALD process of Al<sub>2</sub>O<sub>3</sub> from trimethylaluminum and water on hydrogenated and oxidized Ge(100) surfaces



## INCLUDED FORCEFIELDS (DEVELOPMENT)

See also Included Forcefields (released version)

Description of ReaxFF force fields

Disclaimer: Using these forcefields for systems they have not been explicitly trained against may produce unrealistic results. Please see the full manuscripts for more detailed information.

The force field files used by the SCM version of ReaxFF are compatible with those used by the original ReaxFF code. So if you have the force field information from somewhere else you can just use it (save it in a text file, and select it in ADFinput via the Other... option).

There are currently two major groupings (i.e., the ReaxFF branches) of parameter sets that are intra-transferable with one another: (1) the combustion branch and (2) the aqueous (water) branch. The major difference between these two branches is in the O/H parameters, where the combustion branch focuses on accurately describing water as a gas-phase molecule, and the water branch is targeted at aqueous chemistry.

**AB.ff: (H/O/N/B) Ammonia Borane** M.R.Weismiller, A.C.T. van Duin, J. Lee, R.A. Yetter *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion* *J. Phys. Chem. A* 2010, 114, 5485-5492 (<http://dx.doi.org/10.1021/jp100136c>)

- QM data were generated describing the single and (if relevant) double and triple bond dissociation for all B/N/O/H combinations. These data were used to derive initial ReaxFF bond parameters, and all calculations were performed using DFT with the B3LYP functional and the Pople 6-311G\*\* basis set.
- The training set was then extended with QM data describing angular distortions in a set of small AB-related (AB H<sub>3</sub>N-BH<sub>3</sub>) molecules. These data were used to derive the initial ReaxFF angular parameters.
- The training set was extended with reaction barriers for key reaction steps such as H<sub>2</sub> release from AB, dimerization of H<sub>2</sub>B-NH<sub>2</sub> and reaction energies associated with H<sub>2</sub> release from AB and with AB oxidation.
- Branch: combustion.

**AuCSOH.ff: (Au/C/S/O/H)** J.A. Keith, D. Fantauzzi, T. Jacob, and A.C.T. van Duin *Reactive forcefield for simulating gold surfaces and nanoparticles* *Physical Review B* (2010) 81, 235404-1/235404-8 (<http://dx.doi.org/10.1103/PhysRevB.81.235404>)

- The original Au-Au parameters were extended by three publications:
- Au/O: K. Joshi, A.C.T. van Duin, and T. Jacob Development of a ReaxFF description of gold oxides and initial application to cold welding of partially oxidized gold surfaces *Journal of Materials Chemistry* 20, (2010), 10431-10437 <http://dx.doi.org/10.1039/C0JM01556C>
- Au/C/S/H: T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard Development of interatomic ReaxFF potentials for Au-S-C-H systems *Journal of Physical Chemistry C* 115, (2011), 10315-10322 <http://dx.doi.org/10.1021/jp201496x>

- C/O/H/S: Rahaman, O., van Duin, A. C. T., Goddard, W. A., III, and Doren, D. J. Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization *Journal of Physical Chemistry B* 115 (2011), 249-261 <http://dx.doi.org/10.1021/jp108642r>
- The forcefield does not include Au/N parameters
- Branch: water.

**CHO.ff: (C/H/O) Hydrocarbon oxidation** K.Chenoweth, A.C.T. van Duin, W. A. Goddard *ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation* *J. Phys. Chem. A* 2008, 112, 1040-1053 (<http://dx.doi.org/10.1021/jp709896w>)

- To obtain the H/C/O compound data required to extend the hydrocarbon-training set, DFT calculations were performed on the following systems: (a) dissociation energies for various bonds containing carbon, oxygen, and hydrogen. The ground state structure was obtained through full geometry optimization. Dissociation curves were calculated by constraining only the bond length of interest and re-optimization of the remaining internal coordinates. Optimization was also performed for the various angles and torsions associated with C/H/O interactions.
- Branch: combustion.

**HCONSB.ff: (H/C/O/N/S/B)** M.R. Weismiller, A.C.T. van Duin, J. Lee, and R.A. Yetter, *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion* *J. Phys. Chem. A* (2010), 114, 5485-5492. (<http://dx.doi.org/10.1021/jp100136c>)

- The parameters in this forcefield were extended/improved by two other publications:
- A.M. Kamat, A.C.T. van Duin, and A. Yakovlev *Molecular Dynamics Simulations of Laser-Induced Incandescence of Soot Using an Extended ReaxFF Reactive Force Field*. *Journal of Physical Chemistry A* (2010), 114, 12561-1257 <http://dx.doi.org/10.1021/jp1080302>
- F.Castro-Marcano, A.M. Kamat, M.F. Russo, A.C.T. van Duin, and J.P. Mathews *Combustion of an Illinois No. 6 Coal Char Simulated Using an Atomistic Char Representation and the ReaxFF Reactive Force Field*. *Combustion and Flame* (2012), 159, 23273-1285 <http://dx.doi.org/10.1016/j.combustflame.2011.10.022>
- The C/H/O parameters are the same as in the CHO forcefield, with added S/C, S/H and S/O descriptions. This force field was used in Castro et al, *Combustion and Flame* 2011
- The Boron and Nitrogen parameters are based on (but not identical to) the parameters used in Weismiller et al, *JPC-A* 2010.
- Branch: combustion.

**CuCl-H2O.ff: (Cu/Cl/H/O)** O.Rahaman, A.C.T. van Duin, V.S. Bryantsev, J.E. Mueller, S.D. Solares, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride* *J. Phys. Chem. A* 114 (2010), 3556-3568 (<http://dx.doi.org/10.1021/jp9090415>)

- This forcefield is an extension of: A.C.T. van Duin, V.S. Bryantsev, M.S. Diallo, W.A. Goddard, O. Rahaman, D.J. Doren, D. Raymand, and K. Hermansson *Development and validation of a ReaxFF reactive force field for Cu cation/water interactions and copper metal/metal oxide/metal hydroxide condensed phases* *Journal of Physical Chemistry A* 2010, 114, 9507-9514 <http://dx.doi.org/10.1021/jp102272z>
- Branch: water.

**FeOCHCl.ff: (Fe/O/C/H/Cl)** M.Aryanpour, A.C.T. van Duin, J.D. Kubicki *Development of a Reactive Force Field for Iron-Oxyhydroxide Systems* *J. Phys. Chem. A* 2010, 114, 6298-6307 (<http://dx.doi.org/10.1021/jp101332k>)

- The Cl parameters were published by: O. Rahaman, A.C.T. van Duin, V.S. Bryantsev, J.E. Mueller, S.D. Solares, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride* *J. Phys. Chem. A* 114 (2010), 3556-3568 <http://dx.doi.org/10.1021/jp9090415>

- The initial force field parameters for the Fe-Fe parameters were taken from an earlier force field development project on bulk-iron metal, based on DFT-calculations on antiferromagnetic BCC and FCC. The ReaxFF parameters have not been published yet, however the DFT data can be found in ref 31 of the above mentioned manuscript. The O/H parameters were taken from the ReaxFF bulk water description. The Fe/Fe and O/H parameters were kept fixed to these initial values, whereas the Fe/O parameters were reoptimized against the quantum mechanical results presented in the above mentioned manuscript.
- Detailed information on the force field parameters is given in the supporting information of the above mentioned manuscript.
- Branch: water.

**HE.ff: (C/H/O/N) RDX/High Energy** L.Z. Zhang, A.C.T. van Duin, S.V. Zybin, and W.A. Goddard *Thermal Decomposition of Hydrazines from Reactive Dynamics Using the ReaxFF Reactive Force Field* *Journal of Physical Chemistry B* (2009) 113, 10770-10778 (<http://dx.doi.org/10.1021/jp900194d>)

- Part of this forcefield is also published in: L.Z. Zhang, S.V. Zybin, A.C.T. van Duin, S. Dasgupta, W.A. Goddard, and E.M. Kober Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations *Journal of Physical Chemistry A* (2009) 113, 10619-10640 <http://dx.doi.org/10.1021/jp901353a>
- The parameters of the nitramine ReaxFF are based on a large number of ab initio QM calculations. Over 40 reactions and over 1600 equilibrated molecules have been used; they are designed to characterize the atomic interactions under various environments likely and unlikely high energy each atom can encounter. The training set contains bond breaking and compression curves for all possible bonds, angle and torsion bending data for all possible cases, as well as crystal data.
- Please see the supplemental material from Phys. Rev. Lett. 2003, 91, 098301 for a detailed description of the parameterization of this force field.
- Branch: combustion.

**NaH.ff: (Na/H)** J.G.O. Ojwang, R. Van Santen, G.J. Kramer, A.C.T van Duin, and W.A Goddard *Modeling the sorption dynamics of NaH using a reactive force field* *Journal of Chemical Physics* 2008, 128, 164714 (<http://dx.doi.org/10.1063/1.2908737>)

- This forcefield originally had a typo, defining the H-Na-Na angle twice. The same typo is in table 4 of the publication, but the text clearly mentions that the second line should define Na-H-Na instead.
- Branch: combustion.

**NiCH.ff: (Ni/C/H)** J.E. Mueller, A.C.T. van Duin, and W.A. Goddard III *Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel* *J. Phys. Chem. C* 2010, 114, 4939-4949 (<http://dx.doi.org/10.1021/jp9035056>)

- Branch: combustion.

**SiOH.ff: (Si/O/H)** J.C. Fogarty, H.M. Aktulga, A.Y. Grama, A.C.T. van Duin, S.A. Pandit *A reactive molecular dynamics simulation of the silica-water interface* *J. Chem. Phys.* 2010, 132, 174704 (<http://dx.doi.org/10.1063/1.3407433>)

- This force field was trained to model the interaction of water at the SiO<sub>2</sub> surface, with specific emphasis on proton-transfer reactions. Updated parameters were fitted for all Si/O/H bond, angle, and torsion interactions as well, in addition to the dissociation of a water molecule from a single Si(OH)<sub>4</sub> molecule and reaction energies for the polymerization of Si(OH)<sub>4</sub>
- Branch: water.

**SiC.ff: (Si/C/O/H/N/S)** D.Newsome, D. Sengupta, H. Foroutan, M.F. Russo, and A.C.T. van Duin *Oxidation of Silicon Carbide by O<sub>2</sub> and H<sub>2</sub>O: A ReaxFF Reactive Molecular Dynamics Study, Part I* *Journal of Physical Chemistry* 2012 116, 16111-16121 (<http://dx.doi.org/10.1021/jp306391p>)

- The included forcefield is based on the Newsome reference, with slightly improved parameters by van Duin et al.
- Branch: combustion.

**VOCH.ff: (V/O/C/H)** K.Chenoweth, A.C.T. van Duin, P. Persson, M.J. Cheng, J. Oxgaard, W.A. Goddard *Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts* *J. Phys. Chem. C*, 2008, 112, 14645-14654 (<http://dx.doi.org/10.1021/jp802134x>)

- The ReaxFF force field parameters have been fit to a large quantum mechanics (QM) training set containing over 700 structures and energetics related to bond dissociations, angle and dihedral distortions, and reactions between hydrocarbons and vanadium oxide clusters. In addition, the training set contains charge distributions for small vanadium oxide clusters and the stabilities of condensed-phase systems including V<sub>2</sub>O<sub>5</sub>, VO<sub>2</sub>, and V<sub>2</sub>O<sub>3</sub> in addition to metallic V (V<sub>0</sub>).
- Branch: combustion.

**ZnOH.ff: (Zn/O/H)** D.Raymand, A.C.T. van Duin, M. Baudin, K. Hermansson *A reactive force field (ReaxFF) for zinc oxide* *Surface Science* 2008, 602, 1020-1031 (<http://dx.doi.org/10.1016/j.susc.2007.12.023>)

- updated version published by: D. Raymand, A.C.T. van Duin, D. Spangberg, W.A. Goddard, K. Hermansson *Water adsorption on stepped ZnO surfaces from MD simulation* *Surface Science* 2010, 604, 9-10, 741-752 <http://dx.doi.org/10.1016/j.susc.2009.12.012>
- Based on QM calculations for Zn(s), ZnO(s), and Zn hydroxide clusters [Zn(OH)<sub>2</sub> and O(ZnOH)<sub>2</sub>], ReaxFF parameters were generated for Zn-O and Zn-Zn bond energies and for Zn-O-Zn, O-Zn-O, O-Zn-Zn and Zn-O-H valence angle energies.
- QM calculations were performed for the four crystal polymorphs of the wurtzite, zincblende, rocksalt and caesium chloride structures (the structures are also referred to as h-ZnS, c-ZnS, NaCl and CsCl, respectively).
- Branch: water.

**Al-H<sub>2</sub>O.ff: (Al/H/O)** M.Russo, R. Li, M. Mench, and A.C.T. van Duin *Molecular Dynamic Simulation of Aluminum-Water Reactions Using the ReaxFF Reactive Force Field* *International Journal of Hydrogen Energy* 36 (2011), 5828-5835 (<http://dx.doi.org/10.1016/j.ijhydene.2011.02.035>)

- Branch: water.

**CaSiAlO.ff: (C/H/O/Fe/Cl/Si/Al/Ca)** M.C. Pitman and A.C.T. van Duin *Dynamics of Confined Reactive Water in Smectite Clay-Zeolite Composites* *J. Am. Chem. Soc.*, 2012, 134 (6), 3042-3053 (<http://dx.doi.org/10.1021/ja208894m>)

- Branch: water.

**dispersion/CHONSSi-Ig.ff: (C/H/O/N/S/Si)** L.Liu, Y. Liu, S.V. Zybin, H. Sun, and W.A. Goddard III *ReaxFF-Ig: Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials* *The Journal of Physical Chemistry A*, 2011, 115(40), 11016-11022 (<http://dx.doi.org/10.1021/jp201599t>)

- This forcefield adds London dispersion correction terms to reaxFF, and is optimized for the energetic materials RDX, PETN, TATB, and NM plus graphite, polyethylene, solid carbon dioxide, and solid N<sub>2</sub>, using the low temperature crystal structures to determine the Ig correction parameters.
- Branch: combustion.

**CHOFeAlNiCuS.ff: (C/H/O/Fe/Al/Ni/Cu/S)** O.Rahaman, A.C.T. van Duin, W.A. Goddard III, and D.J. Doren *Development of a ReaxFF reactive force field for glycine and application to solvent effect and tautomerization* *Journal of Physical Chemistry B* 115 (2011), 249-261. (<http://dx.doi.org/10.1021/jp204894m>)

- C/O/H parameters only. The Cu/Fe/Al/Ni parameters are from: Y.K. Shin, H. Kwak, C. Zou, A.V. Vasenkov, and A.C.T. van Duin *Development and Validation of a ReaxFF Reactive Force Field for*

Fe/Al/Ni Alloys: Molecular Dynamics Study of Elastic Constants, Diffusion, and Segregation *J. Phys. Chem. A*, 2012, 116 (49), pp 12163–12174 <http://dx.doi.org/10.1021/jp308507x>

- Not all cross-terms between the two forcefield files are defined, which might cause problems if the system has (for example) C-Cu interactions.
- Branch: water.

**AuSCH\_2011.ff: (Au/S/C/H)** T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard III, *Development of Interatomic ReaxFF Potentials for Au-S-C-H Systems* *J. Phys. Chem. A*, 115, 10315-10322 (2011) (<http://dx.doi.org/10.1021/jp201496x>)

- Branch: combustion.

**AuSCH\_2013.ff: (Au/S/C/H)** Gyun-Tack Bae and Christine M. Aikens *Improved ReaxFF Force Field Parameters for Au-S-C-H Systems* *Journal of Physical Chemistry A* 2013 117 (40), 10438-10446 (<http://dx.doi.org/10.1021/jp405992m>)

- Based upon: T.T. Jarvi, A.C.T. van Duin, K. Nordlund, and W.A. Goddard Development of interatomic ReaxFF potentials for Au-S-C-H systems. *Journal of Physical Chemistry C* 115, (2011), 10315-10322.
- yields improvements for bond bending potential energy surfaces
- aims to agree with DFT geometries of small clusters and gold-thiolate nanoparticles
- Branch: combustion.

**PDMSDecomp.ff: (C/H/O/Si)** K.Chenoweth, S. Cheung, A.C.T. van Duin, W.A. Goddard III, and E.M. Kober *Simulations on the Thermal Decomposition of a Poly(dimethylsiloxane) Polymer Using the ReaxFF Reactive Force Field* *J. Am. Chem. Soc.*, 2005, 127 (19), pp 7192-7202 (<http://dx.doi.org/10.1021/ja050980t>)

- Specialized forcefield, designed to “investigate the failure of the poly(dimethylsiloxane) polymer (PDMS) at high temperatures and pressures and in the presence of various additives”
- Line from the torsion block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: combustion.

**TiOCHNCl.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F)** S.Y. Kim, A.C.T. van Duin, and J.D. Kubicki *Molecular dynamics simulations of the interactions between TiO<sub>2</sub> nanoparticles and water with Na<sup>+</sup> and Cl<sup>-</sup>, methanol, and formic acid using a reactive force field* *Journal of Materials Research / Volume 28 / Issue 03 / 2013*, pp 513-520 (<http://dx.doi.org/10.1557/jmr.2012.367>)

- used for simulating TiO<sub>2</sub>(both rutile and anatase) nanoparticles with water, methanol, and formic acid
- The force field was validated by comparing water dissociative adsorption percentage and bond length between Na-O with density functional theory (DFT) and experimental results
- Branch: water.

**PtCH.ff: (C/H/Pt)** C.F. Sanz-Navarro, P. Astrand, De Chen, M. Ronning, A.C.T. van Duin, T. Jacob, and W.A. Goddard III *Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets* *J. Phys. Chem. A* 112, 1392-1402 (2008) (<http://dx.doi.org/10.1021/jp074806y>)

- Branch: combustion.

**BaYZrCHO.ff: (C/H/O/Ba/Zr/Y)** A.C.T. van Duin, B.V. Merinov, S.S. Jang, and W.A. Goddard III *ReaxFF Reactive Force Field for Solid Oxide Fuel Cell Systems with Application to Oxygen Ion Transport in Yttria-Stabilized Zirconia* *J. Phys. Chem. A*, 112, 3133-3140 (2008) (<http://dx.doi.org/10.1021/jp076775c>)

- Branch: combustion.

**CHONSSiPtZrNiCuCo.ff: (C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co)** K.D. Nielson, A.C.T. van Duin, J. Oxgaard, W.Q. Deng, and W.A. Goddard III *Development of the ReaxFF Reactive Force Field for Describing Transition Metal*

*Catalyzed Reactions, with Application to the Initial Stages of the Catalytic Formation of Carbon Nanotubes* J. Phys. Chem. A, 109, 493-499 (2005) (<http://dx.doi.org/10.1021/jp046244d>)

- Branch: combustion.

**Glycine.ff: (C/H/O/N)** O.Rahaman, A.C.T. van Duin, W.A. Goddard III, and D.J. Doren, *Development of a ReaxFF Reactive Force Field for Glycine and Application to Solvent Effect and Tautomerization* J. Phys. Chem. B, 115, 249-261 (2011) (<http://dx.doi.org/10.1021/jp108642r>)

- Line from the valence angle block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: water.

**SiONH.ff: (C/H/O/N/Si/S)** A.D. Kulkarni, D.G. Truhlar, S.G. Srinivasan, A.C.T. van Duin, P. Norman, and T.E. Schwartzentruber *Oxygen Interactions with Silica Surfaces: Coupled Cluster and Density Functional Investigation and the Development of a New ReaxFF Potential* J. Phys. Chem. C, 2013, 117 (1), pp 258-269 (<http://dx.doi.org/10.1021/jp3086649>)

- Aimed at oxygen interactions with realistic silica surfaces
- Lines from the valence angle block was referring to non-existent atoms from the atomic block and thus was removed.
- Branch: combustion.

**CHOFe.ff: (C/H/O/Fe/Cl/Si/Al)** Chenyu Zou, A.C.T. Van Duin *Investigation of Complex Iron Surface Catalytic Chemistry Using the ReaxFF Reactive Force Field Method* JOM, December 2012, Volume 64, Issue 12, pp 1426-1437 (<http://dx.doi.org/10.1007/s11837-012-0463-5>)

- only the parameters for Fe (and crossterms) differ from the CHOAlSi.ff forcefield
- Branch: water.

**CHOAlSi.ff: (C/H/O/Fe/Cl/Si/Al)** F.Castro-Marcanao, A.C.T. van Duin *Comparison of thermal and catalytic cracking of 1-heptene from ReaxFF reactive molecular dynamics simulations* Combustion and Flame, Volume 160, Issue 4, April 2013, Pages 766-775 (<http://dx.doi.org/10.1016/j.combustflame.2012.12.007>)

- only the parameters for Fe (and crossterms) differ from the CHOFe.ff forcefield
- Branch: water.

**CHOLi.ff: (C/H/O/N/S/Mg/P/Na/Li)** D.Bedrov, G.D. Smith, A.C.T. van Duin *Reactions of Singly-Reduced Ethylene Carbonate in Lithium Battery Electrolytes: A Molecular Dynamics Simulation Study Using the ReaxFF* Journal of Physical Chemistry A, 2012, 116 (11), pp 2978-2985 (<http://dx.doi.org/10.1021/jp210345b>)

- specifically generated for simulating Lithium battery electrolytes
- must be used in combination with the MOLCHARGE keyword to set a charge restraint on Li and CO<sub>3</sub>!
- Branch: water.

**SiOAlLi.ff: (H/O/Si/Al/Li)** B.Narayanan, A.C.T. van Duin, B.B. Kappes, I.E. Reimanis and C.V. Ciobanu *A reactive force field for lithium-aluminum silicates with applications to eucryptite phases* Modelling and Simulation in Materials Science and Engineering 2012 20 015002 (<http://dx.doi.org/10.1088/0965-0393/20/1/015002>)

- Branch: water.

**PdO.ff: (Pd/O)** T.P. Senftle, R.J. Meyer, M.J. Janik and A.C.T. van Duin *Development of a ReaxFF potential for Pd/O and application to palladium oxide formation* The Journal of Chemical Physics 139, 044109 (2013) (<http://dx.doi.org/10.1063/1.4815820>)

- used for studying Oxidation states of Pd nanoparticles, surfaces and bulk configurations with a GCMC method



- Branch: combustion.

**PdH.ff: (Pd/H)** T.P. Senftle, M.J. Janik and A.C.T. van Duin *A ReaxFF Investigation of Hydride Formation in Palladium Nanoclusters via Monte Carlo and Molecular Dynamics Simulations* *The Journal of Physical Chemistry C*, 2014, 118 (9), pp 4967-4981 (<http://dx.doi.org/10.1021/jp411015a>)

- used in combination with a GCMC method
- Branch: combustion.

**Co.ff: (Co)** Xue-Qing Zhang, E. Iype, S.V. Nedeia, A.P.J. Jansen, B.M. Szyja, E.J.M. Hensen, and R.A. van Santen *Site Stability on Cobalt Nanoparticles: A Molecular Dynamics ReaxFF Reactive Force Field Study* *The Journal of Physical Chemistry C*, 2014, 118 (13), pp 6882-6886 (<http://dx.doi.org/10.1021/jp500053u>)

- forcefield was generated using a recently developed Monte Carlo algorithm with simulated annealing.
- Branch: combustion.

**CHONSMgPNaCuCl.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl)** Susanna Monti, Cui Li, and Vincenzo Carravetta *Reactive Dynamics Simulation of Monolayer and Multilayer Adsorption of Glycine on Cu(110)* *J. Phys. Chem. C*, 2013, 117 (10), pp 5221-5228 (<http://dx.doi.org/10.1021/jp312828d>)

- Reactive MD-force field for amino acids on copper
- Branch: water.

**CHOSMoNiLiBFPN.ff: (C/H/O/S/Mo/Ni/Li/B/F/P/N)** Md M. Islam, V.S. Bryantsev, A.C.T. van Duin *ReaxFF Reactive Force Field Simulations on the Influence of Teflon on Electrolyte Decomposition during Li/SWCNT Anode Discharge in Lithium-Sulfur Batteries* *J. Electrochem. Soc.* 2014 volume 161, issue 8, E3009-E3014 (<http://dx.doi.org/10.1149/2.005408jes>)

- forcefield for Electrochemistry in Li-S batteries
- Branch: combustion.

**CHONSSiNaFZr.ff: (C/H/O/N/S/Si/Na/F/Zr)** A.Rahnamoun and A.C.T. van Duin *Reactive Molecular Dynamics Simulation on the Disintegration of Kapton, POSS Polyimide, Amorphous Silica, and Teflon during Atomic Oxygen Impact Using the Reaxff Reactive Force-Field Method* *J. Phys. Chem. A*, 2014, 118 (15), pp 2780-2787 (<http://dx.doi.org/10.1021/jp4121029>)

- comments in the forcefield file: interactions with water and Na+ Fogarty et al. JCP-2010 ; with glycine + C/H/F parameters; Si-F bond/offdiag/angle parameters; Si-S dummy parameters + S-O-H parameters(Yun 2012 Oct8) + H-F bond/offdiag (Jan14 2013 Joon) Jan31: added Zr/O/H/C
- Branch: water.

**TiClOH.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F)** Sung-Yup Kim and A.C.T. van Duin *Simulation of Titanium Metal/Titanium Dioxide Etching with Chlorine and Hydrogen Chloride Gases Using the ReaxFF Reactive Force Field* *J. Phys. Chem. A*, 2013, 117 (27), pp 5655-5663 (<http://dx.doi.org/10.1021/jp4031943>)

- adaptation/evolution of the TiOCHNCl.ff forcefield by Kim, S.-Y. et al.
- Branch: water.

**CHONSSiNaAl.ff: (C/H/O/N/S/Si/Na/Al)** C.Bai, L. Liu, and H. Sun *Molecular Dynamics Simulations of Methanol to Olefin Reactions in HZSM-5 Zeolite Using a ReaxFF Force Field* *J. Phys. Chem. C*, 2012, 116 (12), pp 7029-7039 (<http://dx.doi.org/10.1021/jp300221j>)

- used to simulate methanol to olefin (MTO) reactions in H-ZSM-5 zeolite
- Branch: water.

**undocumented/NiCH.ff: (Ni/C/H/O/N/S/F/Pt/Cl)** Unknown *No Name* Not published (<http://>)

- This forcefield is from april 2009, and is not published

- Branch: combustion.

**LiS.ff: (Li/S)** Md M. Islam, A. Ostadhossein, O. Borodin, A.T. Yeates, W.W. Tipton, R.G. Hennig, N. Kumar, and A.C.T. van Duin *ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials Phys. Chem. Chem. Phys.*, 2015,17, 3383-3393 (<http://dx.doi.org/10.1039/C4CP04532G>)

- Developed for and used to study Sulfur cathode behaviour in Li battery cells
- Branch: combustion.

**CHONSSiPtNiCuCoZrYBa.ff: (C/H/O/N/S/Si/Pt/Ni/Cu/Co/Zr/Y/Ba)** B.V. Merinov, J.E. Mueller, A.C.T. van Duin, Qi An, and W.A. Goddard III *ReaxFF Reactive Force-Field Modeling of the Triple-Phase Boundary in a Solid Oxide Fuel Cell J. Phys. Chem. Lett.*, 2014, 5 (22), pp 4039-4043 (<http://dx.doi.org/10.1021/jz501891y>)

- Force field was developed by combining the YSZ and Ni/C/H descriptions
- From the summary: “The products obtained in our simulations are the same as those in experiment, which indicates that the developed ReaxFF potential properly describes complex physicochemical processes, such as the oxide-ion diffusion, fuel conversion, water formation reaction, coking, and delamination, occurring at the TPB and can be recommended for further computational studies of the fuel/electrode/electrolyte interfaces in a SOFC”
- The Aa atom type is a rename of the Zr atom type, which was defined twice.
- Branch: combustion.

**CHONSSiNaP.ff: (C/H/O/N/S/Si/Na/P)** Bo Zhang, A.C.T. van Duin and J.K. Johnson *Development of a ReaxFF Reactive Force Field for Tetrabutylphosphonium Glycinate/CO2 Mixtures J. Phys. Chem. B*, 2014, 118 (41), pp 12008-12016 (<http://dx.doi.org/10.1021/jp5054277>)

- The forcefield file mentions “Gly with dummy N-P parameters”
- It was developed for studying Carbon dioxide interactions with the ionic liquid tetrabutylphosphonium glycinate, both physical and chemical absorption.
- Several lines from valence angle block were referring to non-existent atoms from the atomic block and thus were removed.
- Branch: combustion.

**CHOLi\_2.ff: (C/H/O/Li)** M.Raju, P. Ganesh, P.R.C. Kent, and A.C.T. van Duin *Reactive Force Field Study of Li/C Systems for Electrical Energy Storage J. Chem. Theory Comput.*, 2015, 11 (5), pp 2156-2166 (<http://dx.doi.org/10.1021/ct501027v>)

- Used for studying Li/C systems with GCMC and MD
- Also contains parameters for “Vi” and “GI”, but these virtual elements are not mentioned in the paper
- Parameters were fitted using a training set consisting, amongst others, of Li binding energies on pristine graphene and graphite, Li migration pathways in graphite and Li dissociation pathways in different hydrocarbons
- The forcefield was validated by a side-by-side comparison of ReaxFF and DFT energies for Li binding on a divacancy, and ReaxFF and DFT ground-state configurations for stage II and stage I stacking in graphite obtained using GCMC simulations
- The forcefield reproduces the in-plane Li ordering as well as the graphite stacking sequence for stage II and stage I compounds
- Branch: water.

**CHONSSiCaCsKsSrNaMgAlCu.ff: (C/H/O/N/S/Si/Ca/Cs/K/Sr/Na/Mg/Al/Cu)** G.M. Psfogiannakis, J.F. McCleerey, E. Jaramillo and A.C.T. van Duin *ReaxFF Reactive Molecular Dynamics Simulation of the Hydra-*



tion of Cu-SSZ-13 Zeolite and the Formation of Cu Dimers J. Phys. Chem. C, 2015, 119 (12), pp 6678-6686 (<http://dx.doi.org/10.1021/acs.jpcc.5b00699>)

- This Cu/Si/Al/O/H forcefield was developed for and used in MD simulations of the hydration of Cu-exchanged SSZ-13 catalyst.
- The force field was developed by merging and expanding previously tested and published ReaxFF force fields for Si/Al/O/H systems and Cu/O/H systems (citations 19-26 of the publication)
- This forcefield is an extension of K.L. Joshi et al 2014, <http://dx.doi.org/10.1039/C4CP02612H>, all non-Cu parameters are the same.
- Branch: water.

**HOSMg.ff: (H/O/S/Mg)** E.Iype, M. Hütter, A.P.J. Jansen, S.V. Nedea and C.C.M. Rindt *Parameterization of a reactive force field using a Monte Carlo algorithm* J. Comput. Chem., 2013, 34: 1143-1154 (<http://dx.doi.org/10.1002/jcc.23246>)

- This forcefield is optimized with a metropolis Monte-Carlo algorithm with simulated annealing to search for the optimum parameters for the ReaxFF force field in a high-dimensional parameter space.
- The optimization is done against a set of quantum chemical data for MgSO<sub>4</sub> hydrates.
- Branch: combustion.

**CHONSMgPNaCuCl\_v2.ff: (C/H/O/N/S/Mg/P/Na/Cu/Cl)** S.Monti, A. Corozzi, P. Fristrup, K.L. Joshi, Yun Kyung Shin, P. Oelschlaeger, A.C.T. van Duin and V. Baronee *Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field* Phys. Chem. Chem. Phys., 2013, 15, 15062-15077 (<http://dx.doi.org/10.1039/C3CP51931G>)

- This forcefield is an extension of CHONSMgPNaCuCl.ff by S. Monti et al., J. Phys. Chem. C, 2013, 117 (10), pp 5221-5228, <http://dx.doi.org/10.1021/jp312828d>
- Developed for peptide and protein simulations
- Branch: water.

**OPt.ff: (O/Pt)** D.Fantauzzi, J. Bandlow, L. Sabo, J.E. Mueller, A.C.T. van Duin and T. Jacob *Development of a ReaxFF potential for Pt-O systems describing the energetics and dynamics of Pt-oxide formation* Phys. Chem. Chem. Phys., 2014, 16, 23118-23133 (<http://dx.doi.org/10.1039/C4CP03111C>)

- Pt-Pt parameters for bulk platinum phases, low & high-index platinum surfaces and nanoclusters.
- O-Pt parameters for bulk platinum oxides, as well as oxygen adsorption and oxide formation on Pt(111) terraces and the {111} and {100} steps connecting them.
- Branch: combustion.

**CHONSMgPNaTiClF.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F)** Stijn Huygh, Annemie Bogaerts, Adri C.T. van Duin and Erik C. Neyts *Development of a ReaxFF reactive force field for intrinsic point defects in titanium dioxide* Computational Materials Science, Volume 95, December 2014, Pages 579-591, ISSN 0927-0256 (<http://dx.doi.org/10.1016/j.commatsci.2014.07.056>)

- Forcefield developed for studying the influence of intrinsic point defects on the chemistry with TiO<sub>2</sub> condensed phases.
- Forcefield seems to be based on TiOCHNCl.ff, <http://dx.doi.org/10.1557/jmr.2012.367>
- Branch: water.

**LiSi.ff: (Li/Si)** A.Ostadossein, E.D. Cubuk, G.A. Tritsarlis, E. Kaxiras, S. Zhanga and A.C.T. van Duin *Stress effects on the initial lithiation of crystalline silicon nanowires: reactive molecular dynamics simulations using ReaxFF* Phys. Chem. Chem. Phys., 2015, 17, 3832-3840 (<http://dx.doi.org/10.1039/C4CP05198J>)

- Branch: combustion.

**CHOFeAlNiCuSCr.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr)** Y.K. Shin, H. Kwak, A.V. Vasenkov, D. Sengupta and A.C.T. van Duin *Development of a ReaxFF Reactive Force Field for Fe/Cr/O/S and Application to Oxidation of Butane over a Pyrite-Covered Cr<sub>2</sub>O<sub>3</sub> Catalyst* ACS Catalysis, 2015, 5 (12), pp 7226-7236 (<http://dx.doi.org/10.1021/acscatal.5b01766>)

- Forcefield optimized for Fe/Cr/O/S
- Branch: water.

**CHOFeAlNiCuSCr\_v2.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr) Ni-O-vacancy** C.Zou et al. *Molecular dynamics simulations of the effects of vacancies on nickel self-diffusion, oxygen diffusion and oxidation initiation in nickel, using the ReaxFF reactive force field* Acta Materialia, Volume 83, 15 January 2015, Pages 102-112 (<http://dx.doi.org/10.1016/j.actamat.2014.09.047>)

- Forcefield optimized for Ni/O, trained with a QM data on Ni, NiO and vacancies
- The non-carbon parameters are the same as in CHOFeAlNiCuSCr\_v3.ff
- Branch: water.

**CHOFeAlNiCuSCr\_v3.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr)** F.Tavazza, T.P. Senftle, C. Zou, C.A. Becker and A.C.T van Duin *Molecular Dynamics Investigation of the Effects of Tip-Substrate Interactions during Nanoindentation* J. Phys. Chem. C, 2015, 119 (24), pp 13580-13589 (<http://dx.doi.org/10.1021/acs.jpcc.5b01275>)

- Combination of the C.ff (condensed carbon) forcefield with Ni/C/O/H parameters
- The non-carbon parameters are the same as in CHOFeAlNiCuSCr\_v2.ff
- Branch: water.

**C.ff: (C) C-2013** S.G. Srinivasan, A.C.T. van Duin and P. Ganesh *Development of a ReaxFF Potential for Carbon Condensed Phases and Its Application to the Thermal Fragmentation of a Large Fullerene* J. Phys. Chem. A, 2015, 119 (4), pp 571-580 (<http://dx.doi.org/10.1021/jp510274e>)

- Forcefield designed for modeling Carbon condensed phases
- Branch: combustion.

**CHONSSiGe.ff: (C/H/O/N/S/Si/Ge)** G.Psofogiannakis and A.C.T van Duin *Development of a ReaxFF reactive force field for Si/Ge/H systems and application to atomic hydrogen bombardment of Si, Ge, and SiGe (100) surfaces* Surface Science 2016, Vol. 646, pp 253-260 (<http://dx.doi.org/10.1016/j.susc.2015.08.019>)

- Forcefield designed for bombardment of Si, Ge and SiGe surfaces with atomic hydrogen.
- Branch: combustion.

**CHONSPtCINi.ff: (C/H/O/N/S/F/Pt/Cl/Ni) Water-Pt-Ni-Nafion** D.Fantauzzi, J.E. Mueller, L. Sabo, A.C.T. van Duin and T. Jacob *Surface Buckling and Subsurface Oxygen: Atomistic Insights into the Surface Oxidation of Pt(111)* ChemPhysChem, 2015, Vol.16: 2797-2802 (<http://dx.doi.org/10.1002/cphc.201500527>)

- extension of the OPt.ff forcefield parameters
- Branch: water.

**CHONSSiPtZrNiCuCoHeNeArKrXe.ff: (C/H/O/N/S/Si/Pt/Zr/Ni/Cu/Co/He/Ne/Ar/Kr/Xe)** A.M. Kamat, A.C.T. van Duin and A. Yakovlev *Molecular Dynamics Simulations of Laser-Induced Incandescence of Soot Using an Extended ReaxFF Reactive Force Field* J. Phys. Chem. A, 2010, 114 (48), pp 12561-12572 (<http://dx.doi.org/10.1021/jp1080302>)

- forcefield designed for the study of Laser-induced incandescence of soot
- Branch: combustion.

**CHOSFCIN.ff: (C/H/O/S/F/Cl/N)** M.A. Wood, A.C.T. van Duin and A. Strachan *Coupled Thermal and Electromagnetic Induced Decomposition in the Molecular Explosive alpha-HMX; A Reactive Molecular Dynamics Study* *J. Phys. Chem. A*, 2014, 118 (5), pp 885-895 (<http://dx.doi.org/10.1021/jp406248m>)

- forcefield designed for studying the combustion of the high-energy material a-HMX
- Branch: combustion.

**Mue2016.ff: (C/H/O/S)** Julian Mueller and Bernd Hartke *ReaxFF Reactive Force Field for Disulfide Mechanochemistry, Fitted to Multireference ab Initio Data;* *J. Chem. Theory Comput.*, 2016, xxx, xxx (<http://dx.doi.org/10.1021/acs.jctc.6b00461>)

- forcefield for studying S-S bond ruptures in mechanophores upon mechanical stress. Ambient conditions, both in gas phase and toluene solvent.
- Branch: combustion.

**CBN.ff: (C/H/B/N)** Sung Jin Pai, Byung Chul Yeo and Sang Soo Han *Reactive force field for the improved design of liquid CBN hydrogen storage materials* *Phys. Chem. Chem. Phys.*, 2016, 18, pp 1818-1827 (<http://dx.doi.org/10.1039/C5CP05486A>)

- forcefield for studying liquid CBN (carbon-boron-nitrogen) hydrogen-storage materials.
- Branch: combustion.

**AgZnO.ff: (C/H/O/N/Si/Cu/Ag/Zn)** A.Lloyd, D. Cornil, A.C.T. van Duin, D. van Duin, R. Smith, S.D. Kenny, J. Cornil and D. Beljonne *Development of a ReaxFF potential for Ag/Zn/O and application to Ag deposition on ZnO* *Surface Science*, 2016, 645, pp 67-73 (<http://dx.doi.org/10.1016/j.susc.2015.11.009>)

- ReaxFF potential for Ag/Zn/O used to study Ag deposition on ZnO.
- Branch: water.

**AlCHO.ff: (Al/C/H/O)** Sungwook Hong and Adri C. T. van Duin *Atomistic-Scale Analysis of Carbon Coating and Its Effect on the Oxidation of Aluminum Nanoparticles by ReaxFF-Molecular Dynamics Simulations* *J. Phys. Chem. C*, 2016, 120 (17), pp 9464-9474 (<http://dx.doi.org/10.1021/acs.jpcc.6b00786>)

- ReaxFF potential for Al/C interactions. Used to investigate carbon coating and its effect on the oxidation of aluminum nanoparticles (ANPs)
- Branch: water.

**CHNa.ff: (C/H/Na)** E.Hjertenaes, A.Q. Nguyen and H. Koch *A ReaxFF force field for sodium intrusion in graphitic cathodes* *Phys. Chem. Chem. Phys.*, 2016, 18, pp 31431-31440 (<http://dx.doi.org/10.1039/C6CP06774C>)

- The force field is applied in hybrid grand canonical Monte Carlo-molecular dynamics (GC-MC/MD) simulations of model systems representative of sodium intrusion in graphitic carbon cathodes used in aluminium electrolysis.
- Branch: combustion.

**CuBTC.ff: (C/H/O/N/S/Mg/P/Na/Cu)** L.Huang, T. Bandosz, K. L. Joshi, A. C. T. van Duin and K. E. Gubbins *Reactive adsorption of ammonia and ammonia/water on CuBTC metal-organic framework: A ReaxFF molecular dynamics simulation* *J. Chem. Phys.*, 2013, 138, 034102 (<http://dx.doi.org/10.1063/1.4774332>)

- The force field was used to study reactive adsorption of NH<sub>3</sub> on the dehydrated CuBTC metal-organic framework.
- Branch: water.

**CHONSMgPNaTiClFAu.ff: (C/H/O/N/S/Mg/P/Na/Ti/Cl/F/Au)** Susanna Monti, Vincenzo Carravetta, and Hans Ågren *Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics* *J. Phys. Chem. Lett.*, 2016, 7 (2), pp 272-276 (<http://dx.doi.org/10.1021/acs.jpcclett.5b02769>)

- The force field was designed to study gold-protein interactions in water.

**HOSiAILi.ff: (H/O/Si/Al/Li)** Alireza Ostadhossein, Sung-Yup Kim, Ekin D. Cubuk, Yue Qi, and Adri C. T. van Duin *Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> Electrodes of Lithium Ion Batteries: ReaxFF Reactive Force Field Modeling* *J. Phys. Chem. A*, 2016, 120 (13), pp 2114-2127 (<http://dx.doi.org/10.1021/acs.jpca.5b11908>)

- Developed for studying the energetics and kinetics of lithiation, as well as Li transportation within the crystalline/amorphous silica and alumina phases.

**CHArHeNeKr.ff: (C/H/Ar/He/Ne/Kr)** Kichul Yoon, A. Rahnamoun, J.L. Swett, V. Iberi, D.A. Cullen, I.V. Vlas-siouk, A. Belianinov, S. Jesse, X. Sang, O.S. Ovchinnikova, A.J. Rondinone, R.R. Unocic, and A.C.T. van Duin *Atomistic-Scale Simulations of Defect Formation in Graphene under Noble Gas Ion Irradiation* *ACS Nano*, 2016, 10 (9), pp 8376-8384 (<http://dx.doi.org/10.1021/acs.nano.6b03036>)

- Developed for studying noble gas ion irradiation of graphene and the subsequent effects of annealing. Lattice defects including nanopores were generated.

**CHO-radiation.ff: (C/H/O)** Roger Smith, K. Jolley, C. Latham, M. Heggie, A van Duin, D. van Duin, Houzheng Wu *A ReaxFF carbon potential for radiation damage studies* *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, Volume 393, 15 February 2017, Pages 49-53, (<http://dx.doi.org/10.1016/j.nimb.2016.11.007>)

- Developed forcefield reproduces the formation energies of many of the defects predicted by the ab initio calculations of energetic impacts and collision cascades in graphite.
- Forcefield reproduces the formation energies of many of the defects predicted by the ab initio calculations and the energy pathways between different defect states, which are important for investigating long term defect evolution.

**HOTiPd.ff: (H/O/Ti/Pd)** Rafik Addou, T.P. Senftle, N. O'Connor, M.J. Janik, A.C.T. van Duin, and M. Batzill *Influence of Hydroxyls on Pd Atom Mobility and Clustering on Rutile TiO<sub>2</sub>(011)-2 x 1* *ACS Nano*, 2014, 8 (6), pp 6321-6333 (<http://dx.doi.org/10.1021/nn501817w>)

- Developed for MC simulations of Pd on TiO<sub>2</sub> surfaces.

**CHONSMgPNaFBLi-e.ff: (C/H/O/N/S/Mg/P/Na/F/B/Li)** M.Islam and A.C.T van Duin *Reductive Decomposition Reactions of Ethylene Carbonate by Explicit Electron Transfer from Lithium: An eReaxFF Molecular Dynamics Study* *J. Phys. Chem. C*, 2016, 120 (48), pp 27128-27134 (<http://dx.doi.org/10.1021/acs.jpcc.6b08688>)

- This forcefield uses the ACKS2 charge model
- This forcefield is an eReaxFF forcefield
- Developed for the study of lithium-ion batteries

**CHOFeAlNiCuSCrSiGe.ff: (C/H/O/Fe/Al/Ni/Cu/S/Cr/Si/Ge)** Y.Zheng, S. Hong, G. Psfogiannakis, S. Datta, B. Rayner, A.C.T. van Duin and R. Engel-Herbert *Modeling and In-situ Probing of Surface Reactions in Atomic Layer Deposition* *ACS Appl. Mater. Interfaces*, 2017, 9 (18), pp 15848-15856 (<http://dx.doi.org/10.1021/acsami.7b01618>)

- Used for studying the ALD process of Al<sub>2</sub>O<sub>3</sub> from trimethylaluminum and water on hydrogenated and oxidized Ge(100) surfaces

## REQUIRED CITATIONS

When you publish results in the scientific literature that were obtained with programs of the ADF package, you are required to include references to the program package with the appropriate release number, and a few key publications. In addition to these general references, references to special features are mandatory, in case you have used them.

### 15.1 General References

The ReaxFF software that SCM makes available is based on the ReaxFF program developed by Adri van Duin.

For calculations with ReaxFF:

1. A.C.T. van Duin, S. Dasgupta, F. Lorant, and W. A. Goddard, *ReaxFF: A reactive force field for hydrocarbons*, *Journal of Physical Chemistry A* 105, 9396-9409 (2001) (<http://dx.doi.org/10.1021/jp004368u>)
2. (a) Chenoweth, A.C.T. van Duin, and W.A. Goddard, *ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation*, *Journal of Physical Chemistry A* 112, 1040-1053 (2008) (<http://dx.doi.org/10.1021/jp709896w>)
11. ReaxFF 2017, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com> Optionally, you may add the following list of authors and contributors: A.C.T. van Duin, W.A. Goddard, M.M. Islam, H. van Schoot, A.L. Yakovlev

The ReaxFF GUI (ReaxFFinput and ADFmovie) has been developed within SCM (with O. Visser as primary developer).

The ReaxFF program has been parallelized, optimized, and extended by SCM (with A.L. Yakovlev as primary developer).

If you use one of the included force fields you must also add the *proper reference for it* (page 41).

Many examples of ReaxFF applications can be found on Prof. van Duin's publication list (<http://www.engr.psu.edu/adri/Publications.aspx>).

### 15.2 Feature References

When you have used force fields or special features, you should include the reference(s) to the implementation.

**Force-bias Monte Carlo (fbMC)** M.J. Mees, G. Pourtois, E.C. Neyts, B.J. Thijsse, A. Stesmans, *Uniform-acceptance force-bias Monte Carlo method with time scale to study solid-state diffusion*, *Physical Review B* 85, 134301 (2012) (<http://dx.doi.org/10.1103/PhysRevB.85.134301>)

**Grand Canonical Monte Carlo (GCMC)** Th.P. Senftle, R.J. Meyer, M.J. Janik and A.C.T. van Duin, *Development of a ReaxFF potential for Pd/O and application to palladium oxide formation*, *J. Chem. Phys.* 139, 044109 (2013) (<http://dx.doi.org/10.1063/1.4815820>)

Th.P. Senftle, A.C.T. van Duin, M.J. Janik, *Determining in situ phases of a nanoparticle catalyst via grand canonical Monte Carlo simulations with the ReaxFF potential*, *Catalysis Communications* \*\*volume 52\*\*, 5 July 2014, Pages 72–77 (<http://dx.doi.org/10.1016/j.catcom.2013.12.001>)

#### Monte-Carlo force-field optimizer (MCFFOptimizer)

5. Iype, M. Huetter, A.P.J. Jansen, S.V. Nedeia, C.C.M. Rindt, *Parameterization of a Reactive Force Field Using a Monte Carlo Algorithm*, *J. Comp. Chem.* 34, 1143-1154 (2013) (<http://dx.doi.org/10.1002/jcc.23246>)

#### ACKS2

20. Verstraelen, P.W. Ayers, V. Van Speybroeck, M. Waroquier, *ACKS2: Atom-Condensed Kohn-Sham DFT Approximated to Second Order* *J. Chem. Phys.* 138, 074108 (2013) (<http://dx.doi.org/10.1063/1.4791569>)

**eReaxFF** M.M. Islam, G. Kolesov, T. Verstraelen, E. Kaxiras, A.C.T. van Duin, *eReaxFF: A Pseudoclassical Treatment of Explicit Electrons within Reactive Force Field Simulations*, *J. Chem.Theory Comput* 12, 3463 (2016) (<http://dx.doi.org/10.1021/acs.jctc.6b00432>)

**ReaxFF Force Field References** When you publish results in the scientific literature that were obtained with one of the included force fields for ReaxFF, including the proper reference for the force field used is mandatory.

- *Forcefields included in the ADF2017 release* (page 41)
- *Forcefields included in the development snapshots* (page 53)

**Reaction Event Detection (ChemTraYzer)** M. Döntgen, M.-D. Przybylski-Freund, L.C. Kröger, W.A. Kopp, A.E. Ismail, K. Leonhard *Automated Discovery of Reaction Pathways, Rate Constants, and Transition States Using Reactive Molecular Dynamics Simulations* (<http://dx.doi.org/10.1021/acs.jctc.5b00201>) *J. Chem.Theory Comput.*, 11 (6), 2517–2524, 2015

## 15.3 External programs and Libraries

Click here for the list of programs and/or libraries used in the ADF package. On some platforms optimized libraries have been used and/or vendor specific MPI implementations.