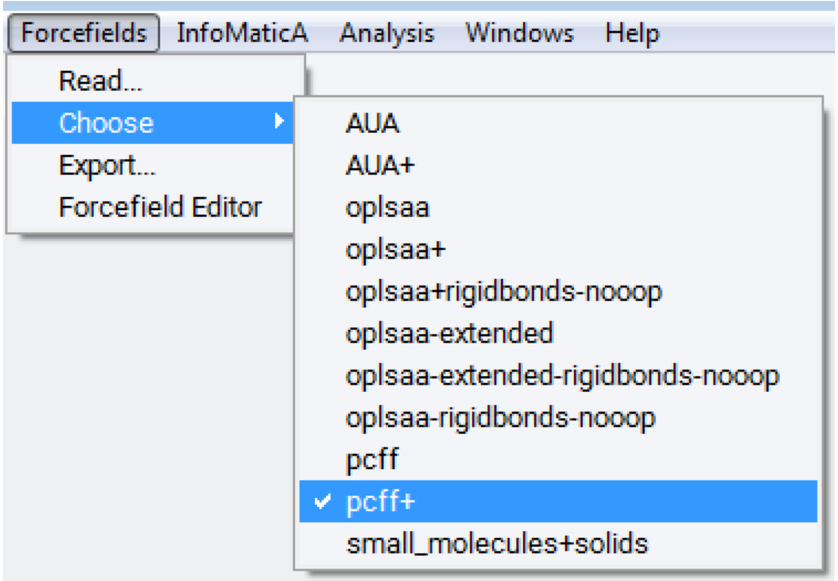
Forcefields

Contents

1 Selecting a Forcefield

To select a specific forcefield, read in a forcefield file from Forcefields >> Read. . . .

One forcefield file can contain different versions, and most likely you want to use the default version.



You can select or verify using a specific variant via Forcefield >> Choose . In this case you want to make sure that you use the additions from MaterialsDesign to pcff:

The initial selection comprises forcefields for:

Organic molecules and polymers

- pcff.frc
- pcff+.frc
- oplsaa.frc
- oplsaa_extended.frc
- oplsaa+.frc
- compass.frc
- compass+.frc (published part)
- AUA.frc
- AUA+.frc
- trappe+.frc
- small_molecules+solids.frc

Inorganic compounds

- inorganic.frc
- cvff.frc (augmented)
- bks.frc
- nacl.frc
- clayff.frc
- clayff-dioctahedral.frc
- clayff-trioctahedral.frc
- comb3.frc
- Si-O_JCP2016-comb3.frc
- AlO_eam_coul.frc
- CeThUNpPuAmCmO_eam_coul.frc
- TaO_eam_coul.frc

Semiconductors

- Tersoff.frc
- SiO2-Si_Munetoh_2007_Tersoff.frc
- StillingerWeber.frc
- ZnCdTeSeHgS_Zhou_2013_StillingerWeber.frc
- REBO.frc

Metallic systems

- Zhou_2004.frc
- Ni_EAM.frc
- ZrH_v4.frc
- md-eam.frc
- EAM_Adams.frc
- AlMg_Adams_1997.frc
- AlCu_Cai_1996.frc
- FeNiCr_Bonny_2011.frc
- AlCo_Mishin_2013.frc
- AlNi_Mishin_2009.frc
- AlTi_Mishin_2003.frc
- MEAM.frc
- AlSiMgCuFe_MEAM.frc
- AuSi_MEAM.frc
- CH_MEAM.frc
- Cu_MEAM.frc
- FeC_MEAM.frc
- FeTiC_MEAM.frc

- Ni_MEAM.frc
- SiC_MEAM.frc
- W_MEAM.frc

3.0

Nist Interatomic Potentials Repository

- Ag-ATVF^Ag.frc
- Ag-YM^Ag.frc
- Al-Fe-MIM^Al-Fe.frc
- Al-LEA^Al-LEA.frc
- Al-MDSL^MDSL.frc
- Al-MIM^Al1.frc
- Al-Mg-LOARH^mg-al-set.frc
- Al-Mg-MIM^Al-Mg.frc
- Al-Pb-LWS^alpb-setfl.frc
- Al-Sm-Mendelev-2014^Al90Sm10_MendelevM_2014.frc
- Al-YM2^Al03.frc
- Al-YM^Al99.frc Au-ATVF^Au.frc
- Au-GRS05^Au-Grochola-JCP05.frc
- Co-PM12^Co_PurjaPun_2012.frc
- Cu-ATVF^Cu.frc
- Cu-Ag-HW^cu_ag_ymwu.frc
- Cu-Ag^CuAg.frc
- Cu-MIM^Cu1.frc
- Cu-MIM^Mendelev_Cu2_2012.frc
- Cu-YM^Cu01.frc
- Cu-Zr^Cu-Zr.frc
- Cu-Zr^Cu-Zr_2.frc
- Fe-ATVF^Fe.frc
- Fe-Cu-Ni-GB^FeCuNi.frc
- Fe-MIM2^Fe_2.frc
- Fe-MIM^Fe_5.frc
- Fe-Ni-Cr-GB-2013^FeNiCr_Bonny_2013_ptDef.frc
- Fe-Ni-Cr-GB^FeNiCr.frc
- Fe-Ni-GB^Fe-Ni.frc
- Fe-P-MIM^Fe-P.frc
- FeC-GJA^Fe-C_Hepburn_Ackland.frc
- Mg-MIM^Mg.frc
- Na-MIM^Na_MendelevM_2014.frc
- Nb-FPW^Nb.frc
- Nb-Ti-Al-Farkas-1996^Farkas_Nb-Ti-Al_1996.frc
- Ni-ATVF^Ni.frc
- Ni-Al-B2^NiAl02.frc
- Ni-Al-Co-YM13^Mishin-Al-Co-2013.frc
- Ni-Al-Co-YM13^Mishin-Ni-Al-Co-2013.frc
- Ni-Al-Co-YM13^Mishin-Ni-Co-2013.frc
- Ni-Al-H-AMB^NiAlH_jea.frc
- Ni-Al-Ni3Al^NiAl.frc
- Ni-Al-YM09^Mishin-Ni-Al-2009.frc
- Ni-MIM-2012^Ni1_Mendelev_2012.frc
- Ni-YM^Ni99.frc
- Ni-Zr-MIM-2012^Ni-Zr_Mendelev_2012.frc
- Ni-Zr-MIM-2014^Ni-Zr_Mendelev_2014.frc
- PdAgH-Hale-2013^PdAgH_HybridPd3Ag.frc
- PdAgH-Hale-2013^PdAgH_MorsePd3Ag.frc
- Ru-MIM^Ru.frc
- Ta-LSAL^newPP1_47-setfl.frc

- Ta-Ravelo-2013^Ta1_Ravelo_2013.frc
- Ta-Ravelo-2013^Ta2_Ravelo_2013.frc
- Ti-Al-RRZ03^Zope-Ti-Al-2003.frc
- Ti-GJA^Ti.frc
- U-Mo-Xe-SKS13^U_Mo_Xe.2013.frc
- V-Fe-MIM^V-Fe.frc
- W-ATVF^W.frc
- Zr-MIM2^Zr_2.frc
- Zr-MIM2^Zr_3.frc
- Zr-MIM^Zr_1.frc

Noble gases

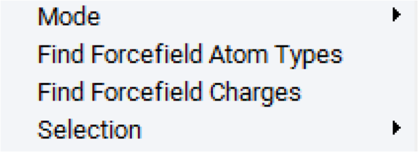
argon_rahman.frc

ReaxFF forcefields

- AuOH.frc
- CHO.frc
- CHON.frc
- CHONSFPtClNi.frc
- FeCHO.frc
- HONB.frc
- VCHO.frc
- ZnOH.frc

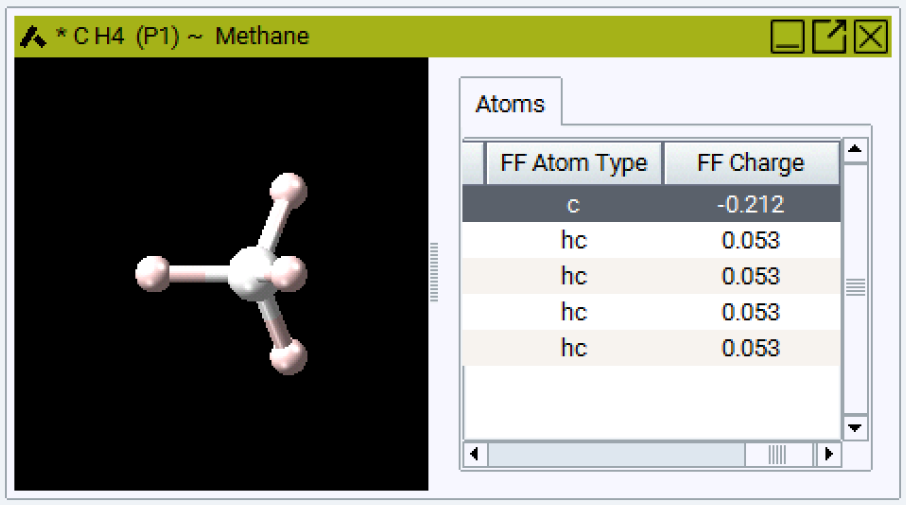
2 Assigning Forcefield Parameters and Charges

Right-click in your model window and use `Find Forcefield Atom types` and `Find Forcefield Charges` to perform the automatic atom type and partial charge assignment.



Note that when using covalent forcefields, it is important to ensure that appropriate bonds and bond orders - single, double, partial-double, triple etc. - have been set in order for correct atom types to be assigned using the forcefield's atom template definitions. Failure to use correct bond orders generally results in atoms with incorrect chemical valence, which can give the misleading impression that a forcefield cannot be used for a given molecule. Therefore, if attempts at atom type assignment result in a warning message indicating that the atom type assignment resulted in unknown atom types, you should first ensure that the chemical structures of the molecules in the model are correct.

You may inspect the assignment by clicking on the Spreadsheet Icon , where atom types are listed in the *FF Atom Type* column (with '?' used to denote any unassigned types). If necessary, the spreadsheet also allows you to change charges and assign any atom type for a selected atom or group of atoms.



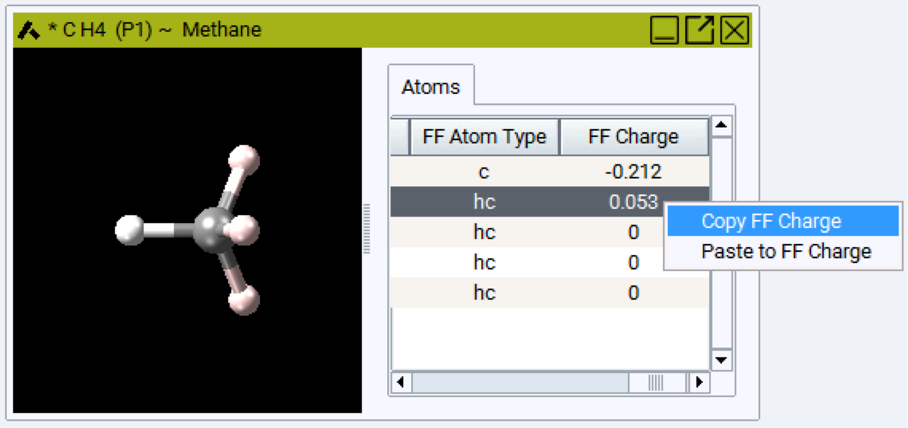
FF Atom Type	FF Charge
c	-0.212
hc	0.053
hc	0.053
hc	0.053
hc	0.053

You can skip the automatic assignment and set all forcefield related values by hand (e.g. to match a publication). In this case, open the spreadsheet and you won't see the columns *FF Atom Type* and *FF Charge*. Insert them by right-clicking in the heading of the spreadsheet and select new columns *FF Atom Type* and *FF Charge*.

You can arrange and sort the atoms in the model and assign atom types to groups by selecting more than one field: The selected fields are highlighted in blue, the active field is white. In the example below you can choose one atom type for all four H atoms in Methane.

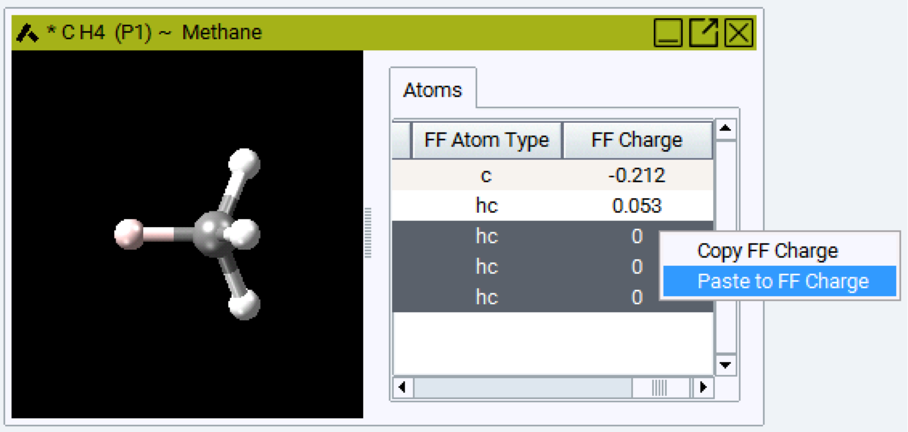
Setting charges is similar:

1. Enter charge for the first atom. Click into field and copy with right-click >> Copy FF charge



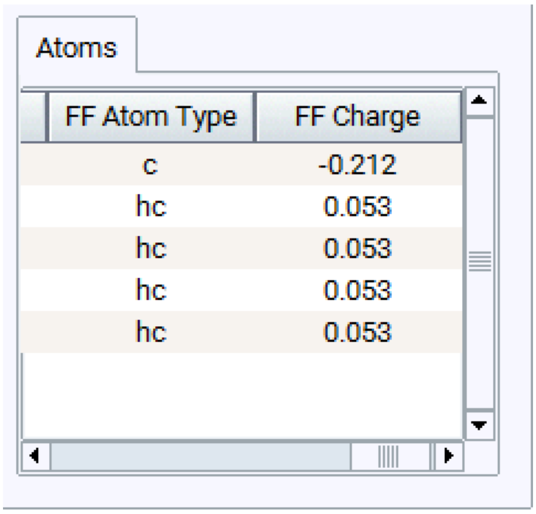
FF Atom Type	FF Charge
c	-0.212
hc	0.053
hc	0
hc	0
hc	0

2. Select remaining atoms with mouse and paste with right-click >> Paste to FF charge



FF Atom Type	FF Charge
c	-0.212
hc	0.053
hc	0
hc	0
hc	0

3. Charge values are copied into the selection



FF Atom Type	FF Charge
c	-0.212
hc	0.053
hc	0.053
hc	0.053
hc	0.053

3 Forcefield Overview

3.1 Organic Molecules and Polymers

We recommend and support the use of pcff+ for all atom molecular dynamics, energy minimization, and related simulations. OPLS-AA, AUA and TraPPE are supplied to use with *MedeA GIBBS* for computationally efficient configurational space sampling and the use of extended atoms.

All the forcefields for organic systems require topological information (such as bonds and bond orders) to determine the atom type and charge for each atom. These forcefields cannot describe the creation or the breaking of bonds.

pcff+.frc:

A significant extension to the *pcff.frc* included with the LAMMPS distribution (see, for example, Sun, Mumby, Maple & Hagler [1]). *pcff+.frc* preserves the ‘cff-series’ ab-initio based parameters for valence interactions (as used in cff91.frc, cff93.frc and pcff.frc). This is supplemented by a substantial refinement of nonbonded parameters based on high quality experimental data for small molecule liquids and gases, together with new parameterizations for selected compounds such as thiophenes. Details are given in the References section at the end of the file.

Ag	Ag	Silver metal
Al	Al	Aluminium metal
Au	Au	Gold metal
Br	Br	bromine ion
Cl	Cl	chlorine ion
Cr	Cr	Chromium metal
Cu	Cu	Copper metal
Fe	Fe	Iron metal
K	K	Potassium metal
Li	Li	Lithium metal
Mo	Mo	Molybdenum metal
Na	Na	Sodium metal

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[1] Huai Sun, Stephen J. Mumby, Jon R. Maple, and Arnold T. Hagler, “An Ab Initio CFF93 All-Atom Force Field for Polycarbonates,” Journal of the American Chemical Society 116, no. 7 (1994): 2978-2987.

Table 1 – continued from previous page

Ni	Ni	Nickel metal
Pb	Pb	Lead metal
Pd	Pd	Palladium metal
Pt	Pt	Platinum metal
Sn	Sn	Tin metal
W	W	Tungsten metal
Ar	ar	Argon
Al	az	aluminium atom in zeolites
Br	br	bromine atom
C	c	generic SP3 carbon
C	c+	C in guanidinium group
C	c-	C in charged carboxylate
C	c1	sp3 carbon with 1 H 3 heavies
C	c2	sp3 carbon with 2 H's, 2 Heavy's
C	c3	sp3 carbon with 3 hHs 1 heavy
C	c3h	sp3 carbon in 3-membered ring with hydrogens
C	c3m	sp3 carbon in 3-membered ring
C	c4h	sp3 carbon in 4-membered ring with hydrogens
C	c4m	sp3 carbon in 4-membered ring
C	c5	sp2 aromatic carbon in 5-membered ring
C	c=	non aromatic end doubly bonded carbon
C	c=1	non aromatic, next to end doubly bonded carbon
C	c=2	non aromatic doubly bonded carbon
C	c_0	carbonyl carbon of aldehydes, ketones
C	c_1	carbonyl carbon of acid, ester, amide
C	c_2	carbonyl carbon of carbamate, urea
C	c_a	general amino acid alpha carbon (sp3)
Ca	ca+	calcium ion
C	cg	sp3 alpha carbon in glycine
C	ci	sp2 aromatic carbon in charged imidazole ring (His+)
Cl	cl	chlorine atom
C	co	sp3 carbon in acetals
C	coh	sp3 carbon in acetals with hydrogen
C	cp	sp2 aromatic carbon
C	cr	C in neutral arginine
C	cs	sp2 aromatic carbon in 5 membered ring next to S
C	ct	sp carbon involved in a triple bond
C	cz	carbonyl carbon of carbonate
D	dw	deuterium in heivy water
F	f	fluorine atom
H	h	generic hydrogen bound to C, Si,or H
H	h*	hydrogen bonded to nitrogen, Oxygen
H	h+	charged hydrogen in cations
H	hb	hydrogen atom in bridging hydroxyl group
H	hc	hydrogen bonded to carbon
He	he	Helium
H	hi	Hydrogen in charged imidazole ring
H	hn	hydrogen bonded to nitrogen
H	hn2	amino hydrogen
H	ho	hydrogen bonded to oxygen
H	ho2	hydroxyl hydrogen
H	hoa	hydrogen atom in terminal hydroxyl group on aluminium
H	hos	hydrogen atom in terminal hydroxyl group on silicon
H	hp	hydrogen bonded to phosphorus

Continued on next page

Table 1 – continued from previous page

H	hs	hydrogen bonded to sulfur
H	hsi	silane hydrogen
H	hw	hydrogen in water
I	i	iodine atom
Kr	kr	Krypton
N	n	generic sp2 nitrogen (in amids))
N	n+	sp3 nitrogen in protonated amines
N	n1	sp2 nitrogen in charged arginine
N	n2	sp2 nitrogen (NH2) in guanidinium group (HN=C(NH2)2)
N	n3m	sp3 nitrogen in 3- membered ring
N	n3n	sp2 nitrogen in 3- membered ring
N	n4	sp3 nitrogen in protonated amines
N	n4m	sp3 nitrogen in 4- membered ring
N	n4n	sp2 nitrogen in 4- membered ring
N	n=	non aromatic end doubly bonded nitrogen
N	n=1	non aromatic, next to end doubly bonded carbon
N	n=2	non aromatic doubly bonded nitrogen
N	n_2	nitrogen of urethane
N	na	sp3 nitrogen in amines
N	nb	sp2 nitrogen in aromatic amines
Ne	ne	Neon
N	nh	sp2 nitrogen in 5 or 6 membered ring
N	nh+	protonated nitrogen in 6 membered ring
N	nho	sp2 nitrogen in 6 membered ring next to a carbonyl
N	ni	nitrogen in charged imidazole ring
N	nn	sp2 nitrogen in aromatic amines
N	np	sp2 nitrogen in 5- or 6- membered ring
N	npc	sp2 nitrogen in 5- or 6- membered ring and with a heavy atom
N	nr	sp2 nitrogen (NH2) in guanidinium group (HN=C(NH2)2)
N	nt	sp nitrogen involved in a triple bond
N	nz	sp3 nitrogen bonded to two atoms
O	o	generic SP3 oxygen
O	o*	oxygen in water
O	o-	partial double oxygen
O	o3e	sp3 oxygen in three membered ring
O	o4e	sp3 oxygen in four membered ring
O	o=	oxygen double bonded to O, C, S, N, P
O	o_1	oxygen in carbonyl group
O	o_2	ester oxygen
O	oah	oxygen atom in terminal hydroxyl group on aluminium
O	oas	oxygen atom between aluminium and silicon
O	ob	oxygen atom in bridging hydroxyl group
O	oc	sp3 oxygen in ether or acetals
O	oe	sp3 oxygen in ester
O	oh	oxygen bonded to hydrogen
O	oo	oxygen in carbonyl group, carbonate only
O	op	sp2 aromatic in 5 membered ring
O	osh	oxygen atom in terminal hydroxyl group on silicon
O	osi	siloxane oxygen
O	oss	oxygen atom betweem two silicons
O	oz	ester oxygen in carbonate
P	p	general phosphorous atom
P	p=	phosphazene phosphorous atom
S	s	sp3 sulfur

Continued on next page

Table 1 – continued from previous page

S	s’	S in thioketone group
S	s-	partial double sulfur
S	s1	sp3 sulfur involved in (S-S) group of disulfides
S	s3e	sulfur in three membered ring
S	s4e	sulfur in four membered ring
S	sc	sp3 sulfur in methionines (C-S-C) group
S	sf	S in sulfonate group
S	sh	sp3 sulfur in sulfhydryl (-SH) group (e.g. cysteine)
Si	si	silicon atom
Si	sio	siloxane silicon
S	sp	sulfur in an aromatic ring (e.g. thiophene)
Si	sz	silicon atom in zeolites
Xe	xe	Xenon
As	as	Arsenic in AsR3
B	b3n	sp2 boron in hexagonal boron nitride
Br	brh	bromine in HBr molecule
C	c0	sp3 carbon with 0 H, 4 heavies
C	c0x	sp3 carbon with 0 H, 4 fluorines
C	c1o	carbon in CO
C	c2=	carbon in CO2 and CS2
C	c3as	sp3 carbon in methyl arsines
C	c3h1	sp3 carbon in 3-membered ring with one hydrogen
C	c3si	sp3 carbon with 3 hydrogens and Si
C	c3o-	carbon in carbonate anion
C	c41o	carbon, sp3, in methanol
C	c43o	carbon, sp3 in secondary alcohols
C	c4h1	sp3 carbon in 4-membered ring with one hydrogen
C	c4o	alpha carbon
C	c0oe	alpha carbon in ether containing tertiary alkyl group, e.g. -C-O-C-R3
C	c1oe	alpha carbon in ether containing secondary alkyl group, e.g. -C-O-CH-R2
C	c2oe	alpha carbon in ether containing primary alkyl group, -C-O-CH2-R
C	c2oz	alpha carbon in carbonates -O(O)C-O-CH2-R
C	c3oe	alpha carbon in methyl containing ethers -C-O-CH3
C	c3oz	alpha carbon in methyl-containing carbonates -O(O)C-O-CH3
C	c4oe	alpha carbon in general ethers -C-O-C- (legacy)
C	c5h	sp3 carbon in 5-membered ring
C	c5h1	sp3 carbon in 5-membered ring with one hydrogen
Cl	cl4	chlorine in ClO4- anion
Cl	clh	chlorine in HCl molecule
C	cpc	alpha/ipso carbon in aromatic ethers -C-O-C-
Cs	Cs+	cesium ion
F	ff	fluorine atom in perfluorinated aliphatics
F	ffp	fluorine atom in perfluorinated aromatics
F	F	fluorine ion
Ge	ge4	generic germanium with four bonds attached
H	h1h	hydrogen in H2
H	h_1p	hydrogen in NH4+
H	hbr	hydrogen in HBr molecule
H	hcl	hydrogen in HCl molecule
H	hhi	hydrogen in HI molecule
H	ho-	hydrogen in hydroxide ion OH-

Continued on next page

Table 1 – continued from previous page

I	I	iodine ion
I	ih	iodine in HI molecule
K	K+	potassium ion
Li	Li+	lithium ion
N	n1o	nitrogen in NO
N	n2o	nitrogen in NO2
N	n2-	nitrogen in amide/imide anion
N	n3b	sp2 nitrogen in hexagonal boron nitride
N	n4o	nitrogen in amine oxides
N	n_3	nitrogen in primary or secondary amide
N	n_3-	nitrogen in NO3- nitrate ion
N	n_30	nitrogen in tertiary amide
N	n_31	nitrogen in secondary amide
N	n_32	nitrogen in primary amide
N	n_4	nitrogen in NH4+
N	n_4c	nitrogen in NR4+
N	na0	sp3 nitrogen in tertiary aliphatic amines
N	na1	sp3 nitrogen in secondary aliphatic amines
N	na2	sp3 nitrogen in primary aliphatic amines (same as na)
N	nbo	sp2 nitrogen in aromatic nitro compounds
Na	Na+	sodium ion
O	o=n	oxygen double bonded to N in aromatic nitro group
O	o1=	oxygen in NO2 and SO2
O	o1=*	oxygen in CO2
O	o1c	oxygen in CO
O	o1c-	oxygen in carbonate anion
O	o1n	oxygen in NO
O	o1n4	oxygen in amine oxides
O	o1o	oxygen in O2
O	o1s-	oxygen in sulfate or sulfonate anion
O	o1n-	oxygen in nitrate ion
O	o2s-	ether oxygen in sulfate anion
O	o_1h	oxygen in carbonyl group of aldehydes
O	o_1r	oxygen in ClO4- anion
O	o_2c	oxygen in carboxylic acids
O	oc	sp3 oxygen in ether or acetals
O	oh-	oxygen in hydroxide ion OH-
P	p6-	phosphorous in phosphate
P	ph3	phosphorous in phosphine
Rb	Rb+	rubidium ion
S	s1=	sulfur in CS2
S	s2=	sulfur in SO2
S	se-	sulfur in sulfate anion

oplsaa+.frc

Based on Jorgensen, Maxwell & Tirado-Rives [2] (oplsaa), supplemented with inclusion of additional parameters derived by various groups (oplsaa_extended), and original work by Materials Design (oplsaa+).

Ar	Ar	Argon atom

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[2] William L Jorgensen, David S Maxwell, and Julian Tirado-Rives, “Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids,” Journal of the American Chemical Society 118, no. 45 (January 1996): 11225-11236.

Table 2 – continued from previous page

C	C	Carbonyl carbon in amides, esters
C	CA	Aromatic carbon
C	CAh1	Aromatic carbon pyridine atom 2
C	CAh2	Aromatic carbon pyridine atom 3
C	CAh3	Aromatic carbon pyridine atom 4
C	CAh4	Aromatic carbon pyrimidine atom 3
C	CAh5	Aromatic carbon pyrimidine atom 4
C	CAh6	Aromatic carbon pyridazine atom 2
C	CAh7	Aromatic carbon pyridazine atom 3
C	CAh8	Aromatic carbon pyrazine
C	CAh9	Aromatic carbon pyrazole
C	CAh0	Aromatic carbon isoxazole
C	CAi1	Aromatic carbon indole atom 4
C	CAi2	Aromatic carbon indole atom 5
C	CAi3	Aromatic carbon indole atom 6
C	CAi4	Aromatic carbon indole atom 7
C	CB	Aromatic carbon indole atom 9
C	CM	sp2 aliphatic carbon
C	CN	aromatic carbon indole atom 8
C	CO	Acetal carbon ROCOR
C	CQ	pyrimidine N-C-N aromatic carbon
C	CR	Aromatic carbon imidazole
C	CRh1	Aromatic carbon oxazole
C	CS	Generic 5-membered ring carbon
C	CSh1	Aromatic carbon pyrrole
C	CSh2	Aromatic carbon furan
C	CSh3	Aromatic carbon indole atom 3
C	CT	sp3 aliphatic carbon
C	CT1	sp3 alpha carbon in nitriles
C	CTEX	Exocyclic sp3 aliphatic carbon in cyclic amine
C	CTfn	Perfluoroalkane carbon
C	CTf4	Tetrafluoromethane carbon
C	CU	Aromatic carbon pyrazole
C	CUh1	Aromatic carbon isoxazole
C	CV	Aromatic carbon imidazole
C	CVh1	Aromatic carbon oxazole
C	CW	sp2 aliphatic carbon
C	CWh1	Aromatic carbon pyrrole
C	CWh2	Aromatic carbon furan
C	CWh3	Aromatic carbon pyrazole
C	CWh4	Aromatic carbon isoxazole
C	CWh5	Aromatic carbon imidazole
C	CWh6	Aromatic carbon oxazole
C	CWh7	Aromatic carbon indole atom 2
C	CZ	sp alkyl nitrile carbon
C	CZ1	sp aryl nitrile carbon
F	F	Fluorine in perfluorinated hydrocarbons
H	H	Amide or amine H(N) hydrogen
H	HA	Aromatic hydrogen
H	HC	Hydrogen bonded to carbon
H	HC1	Hydrogen bonded to carbon in methanol
H	HC2	Hydrogen bonded to carbon in alkenes RH-C= and H2-C=
H	HC3	Hydrogen bonded to carbon in ethers
H	HC4	Hydrogen bonded to carbon next to NR2, NO2, or nitrile

Continued on next page

Table 2 – continued from previous page

H	HC5	alpha alkoxy H in esters
H	HC6	H on alpha carbon of aldehyde and ketone
He	He	Helium atom
H	HEX4	Amine hydrogen in 4-membered cyclic amine (azetidine)
H	HEX5	Amine hydrogen in 5-membered cyclic amine (pyrrolidine)
H	HEX6	Amine hydrogen in 6-membered cyclic amine (piperidine)
H	HW	Hydrogen in TIP3P water
H	HO	Hydrogen bonded to O
H	HS	Hydrogen bonded to S in thiols
Kr	Kr	Krypton atom
N	N	Nitrogen in amides
N	N1	Nitrogen in primary amides
N	N2	Nitrogen in secondary amides
N	N3	Nitrogen in tertiary amides
Ne	Ne	Neon atom
N	NA	Nitrogen in pyrrole
N	NAh2	N-H Nitrogen in pyrazole
N	NAh3	N-H Nitrogen in imidazole
N	NAh4	N-H Nitrogen in indole (atom 1)
N	NB	Nitrogen in pyrazole
N	NBh1	Nitrogen in isoxazole
N	NBh2	Nitrogen in imidazole
N	NBh3	Nitrogen in oxazole
N	NC	Nitrogen in pyridine and diazenes
N	NO	Nitrogen in nitroalkane
N	NT0	Nitrogen in ammonia
N	NT	Nitrogen in primary amines
N	NT2	Nitrogen in secondary amines
N	NT3	Nitrogen in tertiary amines
N	NZ	Nitrogen in nitriles
O	O	Oxygen in amides
O	O1	Oxygen in carboxylate esters
O	O2	Oxygen in aldehydes
O	O3	Oxygen in ketones
O	O4	Oxygen in carboxylic acids RCOOH
O	OH	Oxygen in hydroxyl (OH) group
O	OH2	Oxygen in hydroxyl (OH) group (diols)
O	OH3	Oxygen in hydroxyl (OH) group (triols)
O	OH4	Oxygen in hydroxyl (OH) group (RCOOH)
O	OH5	Oxygen in hydroxyl (OH) group (phenol)
O	ON	Oxygen in nitro group
O	OS	Oxygen in ethers, including acetals
O	OS1	Alkoxy oxygen in esters
O	OW	Oxygen in TIP3P water
S	S	Sulfur in sulfides and disulfides
S	SH	Sulfur in thiols
S	SH1	Sulfur in H2S
Xe	Xe	Xenon atom
C	C1i	aliphatic carbon bonded to N in R4N+
C	C2i	aliphatic carbon bonded to C1i in R4N+
C	CTi	sp3 aliphatic carbon in ionic liquid
F	Fi	Fluorine in ionic liquid anion
H	H1	Hydrogen bonded to C1 in R4N+ cation
N	N2i	Nitrogen bonded to S in triflimide anion

Continued on next page

Table 2 – continued from previous page

N	N4i	Nitrogen in R4N+ cation
O	OYi	Oxygen bonded to S in triflate
S	SY6i	Sulfur in bis triflimide

Trappe+.frc

Martin [3] , Kamath [4] , Stubbs [5] , Wick [6] , Chen [7] , Wick [8] , Martin [9] , Lubna [10] , Maerzke [11]

C	C	Aliphatic
C	CHx-aliphatic	Aliphatic
C	CH4-TraPPE-UA	Molecule CH4-TraPPE-UA
C	CH3-TraPPE-UA	Group CH3-TraPPE-UA-
C	CH2-TraPPE-UA	Group CH2-TraPPE-UA-
C	CH-TraPPE-UA	Group CH-TraPPE-UA-
C	C-TraPPE-UA	Group C-TraPPE-UA-
C	CH2-olef-TraPPE-UA	Group CH2-olef-TraPPE-UA=
C	CH-olef-TraPPE-UA	Group CH-olef-TraPPE-UA=
C	C-olef-TraPPE-UA	Group C-olef-TraPPE-UA=
C	CH-EA-TraPPE-UA	Group CH-EA-TraPPE-UA- for C bonded to O in Ethers and Alcohols
C	CH-(EA)-TraPPE-UA	Group CH-EA-TraPPE-UA- for C bonded to O in Ethers and Alcohols
C	C-EA-TraPPE-UA	Group C-EA-TraPPE-UA- for C bonded to O in Ethers and Alcohols
C	C-(EA)-TraPPE-UA	Group C-EA-TraPPE-UA- for C bonded to O in Ethers and Alcohols
C	C-arom-TraPPE-UA	Aromatic C-arom-TraPPE-UA carbon
C	C-l-arom-TraPPE-UA	Aromatic C-arom-TraPPE-UA carbon linking two rings in condensed units (naphthalene, indane, phenanthrene,..)
C	C-d-arom-TraPPE-UA	Aromatic C-arom-TraPPE-UA carbon linking two rings in diphenyl
C	CH-arom-TraPPE-UA	Aromatic C-arom-TraPPE-UA carbon with one hydrogen
C	CH-aldehyde-TraPPE-UA	C connected to O in aldehydes TraPPE-UA

Continued on next page

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[3] MG Martin and IJ Siepmann, “Transferable Models for Phase Equilibria 1. United-Atom Description of N-Alkanes,” Journal of Physical Chemistry B 102 (1998): 2569.

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[5] John M Stubbs, Jeffrey J Potoff, and J Ilja Siepmann, “Transferable Potentials for Phase Equilibria. 6. United-Atom Description for Ethers, Glycols, Ketones, and Aldehydes,” *Journal of Physical Chemistry B* 108, no. 45 (November 2004): 17596-17605.

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[7] Bin Chen, Jeffrey J Potoff, and J Ilja Siepmann, “Monte Carlo Calculations for Alcohols and Their Mixtures with Alkanes. Transferable Potentials for Phase Equilibria. 5. United-Atom Description of Primary, Secondary, and Tertiary Alcohols,” *Journal of Physical Chemistry B* 105, no. 15 (April 2001): 3093-3104.

[8] Collin D Wick, Marcus G Martin, and J Ilja Siepmann, “Transferable Potentials for Phase Equilibria. 4. United-Atom Description of Linear and Branched Alkenes and Alkylbenzenes,” *Journal of Physical Chemistry B* 104, no. 33 (August 2000): 8008-8016.

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[10] N Lubna, G Kamath, J J Potoff, N Rai, and J I Siepmann, “Transferable Potentials for Phase Equilibria. 8. United-Atom Description for Thiols, Sulfides, Disulfides, and Thiophene,” *Journal of Physical Chemistry B* 109, no. 50 (2005): 24100-24107.

[11] Katie A Maerzke, Nathan E Schultz, Richard B Ross, and J Ilja Siepmann, “TraPPE-UA Force Field for Acrylates and Monte Carlo Simulations for Their Mixtures with Alkanes and Alcohols,” *Journal of Physical Chemistry B* 113, no. 18 (May 7, 2009): 6415-6425.

Table 3 – continued from previous page

C	CH-(aldehyde)-TraPPE-UA	C connected to O in aldehydes TraPPE-UA
C	C-ketone-TraPPE-UA	C connented to O in ketones TraPPE-UA
C	C-(ketone)-TraPPE-UA	C connented to O in ketones TraPPE-UA
C	CH2-cyc5-TraPPE-UA	Group CH2- in a 5-membered cyclic non-aromatic ring
C	CH2-cyc6-TraPPE-UA	Group CH2- in a 6-membered cyclic non-aromatic ring
C	CH-cyc-TraPPE-UA	Group CH- in a 5- or 6-membered cyclic non-aromatic ring
C	C-cyc-TraPPE-UA	Group C- in a 5- or 6-membered cyclic non-aromatic ring
H	H-OH-TraPPE-UA	Hydrogen bonded to O in OH groups
H	H(-OH)-TraPPE-UA	Hydrogen bonded to O in OH groups
H	HA	Aromatic hydrogen
H	UnitedH	ghost H (used also for aromatic in this version)
H	H-SH-TraPPE-UA	H bonded with S in thiols
H	H-pyrrole-TraPPE-UA	H bonded with N in pyrrole
N	N-pyridine-TraPPE-UA	Nitrogen in pyridine
N	N-pyrrole-TraPPE-UA	Nitrogen in pyrrole
N	N-arom-TraPPE-UA	Nitrogen in aromatic rings
O	O-OH-TraPPE-UA	Oxygen in hydroxyl (O-OH-TraPPE-UA) group
O	O(-OH)-TraPPE-UA	Oxygen in hydroxyl (O-OH-TraPPE-UA) group
O	O-ROR-TraPPE-UA	Oxygen in ethers
O	O(ROR)-TraPPE-UA	Oxygen in ethers
O	O-aldehydeketone-TraPPE-UA	Oxygen in aldehydes and ketones TraPPE-UA
O	O-(aldehydeketone)-TraPPE-UA	Oxygen in aldehydes and ketones TraPPE-UA
S	S	Sulfur
S	S-thiol-TraPPE-UA	Sulfur in thiols
S	S-sulfide-TraPPE-UA	Sulfur in sulfides
S	S-disulfide-TraPPE-UA	Sulfur in disulfides
S	S-thiophene-TraPPE-UA	Sulfur in thiophene

compass+.frc - The Published Part of COMPASS

Supplied for consistency with the LAMMPS distribution. General use of this forcefield is deprecated, as the forcefield is not maintained. [12] Contains the collection of compass parameters in their original published

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[12] H Sun, "COMPASS: an Ab Initio Force-Field Optimized for Condensed-Phase -Overview with Details on Alkane and Benzene Compounds," *Journal of Physical Chemistry B* 102, no. 38 (September 1998): 7338-7364.

form. compass+.frc includes subsequently published corrections.

Cvff.frc

Supplied for consistency with the LAMMPS distribution. General use of this forcefield is deprecated. [13]

Cff91.frc

Supplied for consistency with the LAMMPS distribution. General use of this forcefield is deprecated. [14]

Cff93.frc

Supplied for consistency with the LAMMPS distribution. General use of this forcefield is deprecated. [15]

3.2 Inorganic Compounds

We don’t make overall recommendations for inorganic forcefields, because the local coordination of inorganic systems varies widely, and the transferability of forcefield terms cannot be assumed from one compound to another. The scope and applicability of forcefields for inorganics are best discerned through reference to their original derivation. These forcefields don’t require bonds.

inorganic.frc

Compiled by Woodley, Battle, Gale & Catlow [16], Xia [17] for use in inorganic crystal structure prediction.

Ag	Ag1+	
Ag	Ag3+	
Al	Al3+	
Ba	Ba2+	
Ca	Ca2+	
Cd	Cd2+	
Ce	Ce4+	
Co	Co2+	
Co	Co3+	
Cr	Cr3+	
Cu	Cu1+	
Fe	Fe2+	
Fe	Fe3+	
Ge	Ge4+	

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[13] Jörg-Rüdiger Hill, Clive M Freeman, and Lalitha Subramanian, “Use of Force Fields in Materials Modeling,” in Reviews in Computational Chemistry, ed. by Kenny B Lipkowitz and Donald B Boyd, vol. 16, (Hoboken, NJ, USA: John Wiley & Sons, Inc., 2000), 141-216.

[14] J R Maple, M J Hwang, T P Stockfisch, U Dinur, M Waldman, et al., “Derivation of Class II Force Fields. I. Methodology and Quantum Force Field for the Alkyl Functional Group and Alkane Molecules,” Journal of Computational Chemistry 15, no. 2 (February 1994): 162-182; M J Hwang, T P Stockfisch, and A T Hagler, “Derivation of Class II Force Fields. 2. Derivation and Characterization of a Class II Force Field, CFF93, for the Alkyl Functional Group and Alkane Molecules,” Journal of the American Chemical Society 116, no. 6 (1994): 2515-2525.

[15] J R Maple, M J Hwang, T P Stockfisch, U Dinur, M Waldman, et al., “Derivation of Class II Force Fields. I. Methodology and Quantum Force Field for the Alkyl Functional Group and Alkane Molecules,” Journal of Computational Chemistry 15, no. 2 (February 1994): 162-182; M J Hwang, T P Stockfisch, and A T Hagler, “Derivation of Class II Force Fields. 2. Derivation and Characterization of a Class II Force Field, CFF93, for the Alkyl Functional Group and Alkane Molecules,” Journal of the American Chemical Society 116, no. 6 (1994): 2515-2525.

[16] S.M. Woodley, P.D. Battle, J D Gale, and C Richard A Catlow, “The Prediction of Inorganic Crystal Structures Using a Genetic Algorithm and Energy Minimisation,” Physical Chemistry Chemical Physics 1, no. 10 (1999): 2535-2542.

[17] Xin Xia, “Computational Modelling Study of Yttria-Stabilized Zirconia,” (University College London, 2010).

Table 4 – continued from previous page

K	K1+	
La	La3+	
Mg	Mg2+	
Mn	Mn2+	
Mn	Mn4+	
Na	Na1+	
Nb	Nb5+	
Ni	Ni2+	
O	O2-	
O	O12-	
O	O22-	
Pb	Pb1+	
Po	Po4+	
Pr	Pr3+	
Rb	Rb1+	
Si	Si4+	
Sn	Sn4+	
Sr	Sr2+	
Ta	Ta2+	
Tl	Tl3+	
Ti	Ti3+	
Ti	Ti4+	
U	U2+	
V	V2+	
V	V3+	
V	V4+	
Y	Y3+	
Zn	Zn2+	
Zr	Zr2+	

bks.frc

Derived by van Beest, Kramer & van Santen [18] to provide a description of structural and vibrational properties for framework structure materials based on two-body (i.e. without explicit angle terms).

Al	Al	
O	O	
P	P	
Si	Si	

CVFF_aug.frc

This forcefield was developed by Behnam Vessal using a methodology similar to that employed by van Beest, to create a broad two-body (i.e. without explicit angle terms) description of framework structured materials able to support extra framework atoms. [19]

H	h	Hydrogen bonded to C. Masses from CRC 1973/74 pages B-250.

Continued on next page

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[18] B W H van Beest, G J Kramer, and R A van Santen, "Force Fields for Silicas and Aluminophosphates Based on Ab Initio Calculations," Physical Review Letters 64, no. 16 (April 1990): 1955-1958.

[19] Jö rg-R diger Hill, Clive M Freeman, and Lalitha Subramanian, "Use of Force Fields in Materials Modeling," in Reviews in Computational Chemistry, ed. by Kenny B Lipkowitz and Donald B Boyd, vol. 16, (Hoboken, NJ, USA: John Wiley & Sons, Inc., 2000), 141-216.

Table 5 – continued from previous page

H	d	General Deuterium
H	hn	Hydrogen bonded to N
H	ho	Hydrogen bonded to O
H	hp	Hydrogen bonded to P
H	hs	Hydrogen bonded to S
H	h*	Hydrogen in water molecule
H	h$	Hydrogen atom for automatic parameter assignment
L	lp	Lone Pair
L	lp	Lone Pair
H	h+	Charged hydrogen in cations
H	hc	Hydrogen bonded to carbon
H	hi	Hydrogen in charged imidazole ring
H	hw	Hydrogen in water
D	dw	Deuterium in heivy water
C	c	Sp3 aliphatic carbon
C	cg	Sp3 alpha carbon in glycine
C	c’	Sp2 carbon in carbonyl (C=O) group
C	c*	Carbon in carbonyl group, non_amides
C	c”	Carbon in carbonyl group, non_amides
C	cp	Sp2 aromatic carbon (partial double bonds)
C	cr	Carbon in guanidinium group (HN=C(NH2)2)
C	c+	C in guanidinium group
C	c-	Carbon in charged carboxylate (COO-) group
C	ca	General amino acid alpha carbon (sp3)
C	c3	Sp3 carbon in methyl (CH3) group
C	cn	Sp3 Carbon bonded to N
C	c2	Sp3 carbon bonded to 2 H’s, 2 heavy atoms
C	c1	Sp3 carbon bonded to 1 H, 3 Heavy atoms
C	c5	Sp2 aromatic carbon in five membered ring
C	cs	Sp2 carbon involved in thiophene
C	c=	Non aromatic end doubly bonded carbon
C	c=1	Non aromatic, next to end doubly bonded carbon
C	c=2	Non aromatic doubly bonded carbon
C	ct	Sp carbon involved in triple bond
C	ci	Sp2 aromatic carbon in charged imidazole ring (His+)
C	c$	Carbon atom for automatic parameter assignment
C	co	Sp3 carbon in acetals
C	c3m	Sp3 carbon in 3-membered ring
C	c4m	Sp3 carbon in 4-membered ring
C	coh	Sp3 carbon in acetals with hydrogen
C	c3h	Sp3 carbon in 3-membered ring with hydrogens
C	c4h	Sp3 carbon in 4-membered ring with hydrogens
C	ci	Sp2 aromatic carbon in charged imidazole ring (His+)
N	n	Sp2 nitrogen with 1 H, 2 heavy atoms (amide group)
N	no	Sp2 nitrogen in nitro group
N	n2	Sp2 nitrogen (NH2 in the guanidinium group (HN=C(NH2)2))
N	np	Sp2 aromatic nitrogen (partial double bonds)
N	n3	Sp3 nitrogen with three substituents
N	n4	Sp3 nitrogen with four substituents
N	n=	Non aromatic end double bonded nitrogen
N	n=1	Non aromatic, next to end doubly bonded carbon
N	n=2	Non aromatic doubly bonded nitrogen
N	nt	Sp nitrogen involved in triple bond
N	nz	Sp nitrogen in N2

Continued on next page

Table 5 – continued from previous page

N	n1	Sp2 nitrogen in charged arginine
N	ni	Sp2 nitrogen in a charged imidazole ring (HIS+)
N	n$	Nitrogen atom for automatic parameter assignment
N	na	Sp3 nitrogen in amines
N	n3m	Sp3 nitrogen in 3- membered ring
N	n4m	Sp3 nitrogen in 4- membered ring
N	n3n	Sp2 nitrogen in 3- membered ring
N	n4n	Sp2 nitrogen in 4- membered ring
N	nb	sp2 nitrogen in aromatic amines
N	nn	sp2 nitrogen in aromatic amines
N	npc	sp2 nitrogen in 5- or 6- membered ring bonded to a heavy atom
N	nh	sp2 nitrogen in 5-or 6- membered ring with hydrogen attached
N	nho	sp2 nitrogen in 6- membered ring next to a carbonyl group and with a hydrogen
N	nh+	protonated nitrogen in 6- membered ring with hydrogen attached
N	n+	sp3 nitrogen in protonated amines
N	nr	sp2 nitrogen (NH2) in guanidinium group (HN=C(NH2)2)
O	o’	Oxygen in carbonyl (C=O) group
O	o	sp3 oxygen in ether or ester groups
O	o-	Oxygen in charged carboxylate (COO-) group
O	oh	Oxygen in hydroxyl (OH) group
O	o*	Oxygen in water molecule
O	op	Oxygen in aromatic rings. e.g. furan
O	of	Oxygen in
O	o$	Oxygen atom for automatic parameter assignment
O	oc	sp3 oxygen in ether or acetals
O	oe	sp3 oxygen in ester
O	o3e	sp3 oxygen in three membered ring
O	o4e	sp3 oxygen in four membered ring
S	s	Sulfur in methionine (C-S-C) group
S	s1	Sulfur involved in S-S disulfide bond
S	sh	Sulfur in sulfhydryl (-SH) group
S	sp	Sulfur in thiophene
S	s’	Sulfur in thioketone (>C=S) group
S	s$	Sulfur atom for automatic parameter assignment
S	sc	sp3 sulfur in methionines (C-S-C) group
S	s3e	Sulfur in three membered ring
S	s4e	Sulfur in four membered ring
S	s-	Sulfur bonded to something then bonded to another partial double O or S
P	p	General phosphorous atom
P	p$	Phosphorous atom for automatic parameter assignment
Ca	ca+	Calcium ion - Ca++, mass = mass of Ca - 2*electron mass.
F	f	Fluorine bonded to a carbon
Cl	cl	Chlorine bonded to a carbon
Br	br	Bromine bonded to a carbon
I	i	Covalently bound Iodine
Si	si	Silicon atom (General)
H	nu	NULL atom for relative free energy
Cl	Cl	Chloride ion Cl-
Br	Br	Bromide ion Br-
Na	Na	Sodium metal

Continued on next page

Table 5 – continued from previous page

Ar	ar	Argon
Si	sz	Silicon atom in zeolites
Si	sy	Tetrahedral Silicon atom in Clays
O	oz	Oxygen atom in zeolites
O	oy	Oxygen atom in Clays
Al	az	Tetrahedral Aluminum atom in zeolites
Al	ay	Octahedral Aluminum atom in Clays
Al	ayt	Tetrahedral Aluminum atom to be used with oy
P	pz	Phosphorous atom in zeolites
P	py	Phosphorous atom to be used with oy
Ga	ga	Gallium atom in zeolites
Ge	ge	Germanium atom in zeolites
Ti	tioc	Titanium (Octahedral) in zeolites
Ti	ti4c	Titanium (Octahedral) to be used with oy
Ti	titd	Titanium (Tetrahedral) in zeolites
Li	li+	Lithium ion in zeolites
Li	lic+	Lithium ion to be used with oy in Clays
Li	lioh	Lithium ion in water to be used with o*
Na	na+	Sodium ion in zeolites
Na	nac+	Sodium ion in Clays
Na	naoh	Sodium ion in water to be used with o*
K	k+	Potassium ion in zeolites
K	koh	Potassium ion in water to be used with o*
Rb	rb+	Rubidium ion in zeolites
Cs	cs+	Cesium ion in zeolites
N	nh4+	United atom type for ammonium ion to be used with oy
Mg	mg2+	Magnesium ion in zeolites
Mg	mg2c	Octahedral Magnesium ion in Clays
Mn	mn4c	Manganese (IV) ion to be used with oy in Clays
Mn	mn3c	Manganese (III) ion to be used with oy in Clays
Co	co2c	Cobalt (II) ion to be used with oy in Clays
Ni	ni2c	Nickel (II) ion to be used with oy in Clays
Ca	ca2+	Calcium ion in zeolites
Ca	ca2c	Calcium ion to be used with oy in Clays
Sr	sr2c	Strontium ion to be used with oy in Clays
Ba	ba2+	Barium ion in zeolites
Cu	cu2+	Copper(II) ion in zeolites
Fe	fe2c	Octahedral Fe(II) ion in clays
F	f-	Fluoride ion in zeolites
Be	beoh	Beryllium (II) in water to be used with o*
F	foh	Fluoride ion in water to be used with o*
Cl	cl-	Chloride ion in zeolites
Cl	cloh	Chloride ion in water to be used with o*
Cl	cly-	Chloride ion to be used with oy in Clays
Br	br-	Bromide ion in zeolites
I	i-	Iodide ion in zeolites
S	so4	Sulfur in sulphate ion to be used with oz
S	so4y	Sulfur in sulphate ion to be used with oy in Clays
H	hocl	Hydrogen in hydroxyl group in Clays
Pd	pd2+	Palladium(II)
V	vy	Tetrahedral Vanadium to be used with oy
Al	al	Aluminium metal
Na	Na	Sodium metal
Pt	Pt	Platinum metal

Continued on next page

Table 5 – continued from previous page

Pd	Pd	Palladium metal
Au	Au	Gold metal
Ag	Ag	Silver metal
Sn	Sn	Tin metal
K	K	Potassium metal
Li	Li	Lithium metal
Mo	Mo	Molybdenum metal
Fe	Fe	Iron metal
W	W	Tungsten metal
Ni	Ni	Nickel metal
Cr	Cr	Chromium metal
Cu	Cu	Copper metal
Pb	Pb	Lead metal

Nacl.fr

This forcefield provides an illustration of the incorporation of a general inorganic forcefield description in the *MedeA* environment framework.

Na	Na1+	sodium atom
Cl	Cl1-	chlorine atom

Clayff.frc clayff-dioctahedral.frc clayff-trioctahedral.frc

H	h*	water hydrogen
H	ho	H hydroxyl hydrogen
O	o*	water oxygen
O	oh	hydroxyl oxygen
O	ob	Basal bridging oxygen
O	oa	Applical bridging oxygen
Si	st	Silicon in SiO2
Al	ao	Aluminium in the octahedral sheet
Al	at	Aluminium in Zeolites
Mg	mgo	Magnesium in the octahedral sheet
Ca	cao	Calcium in the octahedral sheet
Fe	feo	iron in the octahedral sheet
Li	lio	Lithium in the octahedral sheet
O	obss	bridging oxygen with double substitution
O	obts	bridging oxygen with tetrahedral substitution
O	obos	bridging oxygen with octahedral substitution
O	ohs	hydroxyl oxygen with substitution
Ca	cah	hydroxide calcium
Mg	mgh	hydroxide magnesium
Na	Na	Sodium ion
K	K	Potassium ion
Cs	Cs	Cs+ ion
Ca	Ca	Ca2+ ion
Ba	Ba	Ba2+ ion
Cl	Cl	Cl- ion

AlO_eam_coul.frc TaO_eam_coul.frc CeThUNpPuAmCmO_eam_coul.frc

These forcefields are known as the Streitz-Mintmire or charge-transfer ionic (CTIP) potentials [20] which combine EAM and Coulomb (charges described via Slater type orbitals instead of point charges) forcefields along with variable charge equilibration.

AlO_eam_coul.frc

Al	Al	
O1	O1	

TaO_eam_coul.frc

Ta	Ta	
O2	O2	

CeThUNpPuAmCmO_eam_coul.frc

Ce	Ce	
Th	Th	
U	U	
Np	Np	
Pu	Pu	
Am	Am	
Cm	Cm	
O	O	

comb3.frc Si-O_JCP2016-comb3.frc

The 3rd generation charge-optimized many-body (COMB3) [21] forcefields are improvements over the previous generations of COMB forcefields. COMB3 contains an advanced bond order term for describing complex chemical reactions (bond breaking and formation), Coulomb with charge density described with Slater-type orbitals, and variable charge equilibration (atomic charges automatically assigned based on atomic surroundings).

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[20] F. H. Streitz and J. W. Mintmire, “Electrostatic potentials for metal-oxide surfaces and interfaces” Phys. Rev. B 50, 11996

[21] T. Liang, T.-R. Shan, Y.-T. Cheng, B. D. Devine, M. Noordhoek, Y. Li, Z. Lu, S. R. Phillpot, and S. B. Sinnott, Mat. Sci. & Eng: R 74, 255-279 (2013).

comb3.frc

Ti	Ti	Titanium
H	H	Hydrogen
C	C	Carbon
N	N	Nitrogen
O	O	Oxygen
Cu	Cu	Copper
Zn	Zn	Zinc
Zr	Zr	Zirconium
Si	Si	Silicon
Ti	Ti	Titanium
Al	Al	Aluminum
Ni	Ni	Nickel
Mo	Mo	Molybdenum
S	S	Sulfur
Pt	Pt	Platinum
Au	Au	Gold

Si-O_JCP2016-comb3.frc

O	O	Oxygen
Si	Si	Silicon

3.3 Semiconductors

Forcefields for semiconductor materials. These forcefields don't require bonds.

StillingerWeber.frc ZnCdTeSeHgS_Zhou_2013_StillingerWeber.frc

Stilllinger-Weber forcefields that allow for the simulation of various crystalline and amorphous solids. This forcefield uses an explicit angular term to assess nearest neighbor coordination (to include three-body forces) based on the local environment of simulated atoms [22].

StillingerWeber.frc

Cd	Cd	cadmium
Ga	Ga	gallium
N	N	nitrogen
Si	Si	silicon
Te	Te	tellurium

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[22] Frank H Stillinger and Thomas A Weber, "Computer Simulation of Local Order in Condensed Phases of Silicon," Physical Review B 31, no. 8 (1985): 5262-5271; A. Bò rò and A. Serra, "On the Atomic Structures, Mobility and Interactions of Extended Defects in GaN: Dislocations, Tilt and Twin Boundaries," Philosophical Magazine 86, no. 15 (2006): 2159-2192.

ZnCdTeSeHgS_Zhou_2013_StillingerWeber.frc

Cd	Cd	cadmium
Zn	Zn	zinc
Te	Te	tellurium
Se	Se	selenium
Hg	Hg	mercury
S	S	sulfur

Tersoff.frc SiO2-Si_Munetoh_2007_Tersoff.frc

Tersoff forcefields that allow for the simulation of various crystalline and amorphous solids. This forcefield uses a bond order term to assess nearest neighbor coordination (to include three-body forces) based on the local environment of simulated atoms. [23]

Tersoff.frc

C	C	carbon
Ga	Ga	gallium
Ge	Ge	germanium
N	N	nitrogen
Si	Si	silicon, final parameters
Si	Si(B)	silicon, original parameters
Si	Si(C)	silicon, second set of parameters
O	O	oxygen atom

SiO2-Si_Munetoh_2007_Tersoff.frc

Si	Si	silicon, final parameters
O	O	oxygen atom

REBO.frc

1st generation reactive bond order (REBO)[#30_24]_ forcefield closely related to Tersoff forcefields. It allows for simulations of Si with Cl, with Ar described via Moliere forcefield.

Si	Si	silicon
Cl	Cl	chlorine
Ar	Ar	argon

3.4 Metallic

The forcefields in this section don't require bonds during atom type assignment and allow to study of metallic systems using the EAM (embedded atom model) description pioneered by Mike Baskes and others.

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[23] J Tersoff, "New Empirical Approach for the Structure and Energy of Covalent Systems," Physical Review B 37, no. 12 (1988): 6991-7000; J Tersoff, "Empirical Interatomic Potential for Silicon with Improved Elastic Properties," Physical Review B 38, no. 14 (1988): 9902-9905; J Tersoff, "Modeling Solid-State Chemistry: Interatomic Potentials for Multicomponent Systems," Physical Review B 39, no. 8 (1989): 5566-5568; J Tersoff, "Erratum: Modeling Solid-State Chemistry: Interatomic Potentials for Multicomponent Systems," Physical Review B 41, no. 5 (1990): 3248-3248; "Modelling of Compound Semiconductors: Analytical Bond-Order Potential for Gallium, Nitrogen and Gallium Nitride," Journal of Physics: Condensed Matter 15, no. 32 (2003): 5649.

As noted above, the variability in local coordination inherent in inorganic systems (as opposed to organic systems) dictates that the creation of transferable forcefield descriptions is challenging for such systems. Hence, for each of the inorganic and metallic forcefield descriptions we recommend that the original references are consulted in order to assess the applicability of these descriptions to a particular system.

Zhou_2004.frc

This forcefield provides support for the following set of atoms and alloys composed of mixtures of these atoms. Zhou [25], with additions from Francis [26]

Ag	Ag	silver
Al	Al	aluminum
Au	Au	gold
Co	Co	cobalt
Cu	Cu	copper
Fe	Fe	iron
Mg	Mg	magnesium
Mo	Mo	molybdenum
Ni	Ni	nickel
Pb	Pb	lead
Pd	Pd	palladium
Pt	Pt	platinum
Ta	Ta	tantalum
Ti	Ti	titanium
W	W	tungsten
Zr	Zr	zirconium

EAM_Adams.frc

Li, Siegel, Adams, and Liu: [27]

Al	Al	aluminum
Au	Au	gold
Cu	Cu	copper
Ni	Ni	nickel
Pd	Pd	palladium
Pt	Pt	platinum
Ta	Ta	tantalum

Ni_EAM.frc

Mishin [28] , Ackland [29]

Ni	Ni	Nickel

---

[25] X Zhou, R Johnson, and H Wadley, “Misfit-Energy-Increasing Dislocations in Vapor-Deposited CoFe/NiFe Multilayers,” Physical Review B 69, no. 14 (April 2004).

[26] M F Francis, M N Neurock, X W Zhou, J J Quan, H N G Wadley, et al., “Atomic Assembly of Cu/Ta Multilayers: Surface Roughness, Grain Structure, Misfit Dislocations, and Amorphization,” Journal of Applied Physics 104, no. 3 (2008): 034310.

[27] Youhong Li, Donald J Siegel, James Adams, and Xiang-Yang Liu, “Embedded-Atom-Method Tantalum Potential Developed by the Force-Matching Method,” Physical Review B 67, no. 12 (2003).

[28] Yuri Mishin and Diana Farkas, “Atomistic Simulation of Point Defects and Diffusion in B2 NiAl Part1: Point Defect Energetics,” Philosophical Magazine A 75, no. 1 (1997): 169-185; Yuri Mishin and Diana Farkas, “Atomistic Simulation of Point Defects and Diffusion in B2 NiAl Part2: Diffusion Mechanisms,” Philosophical Magazine A 75, no. 1 (1997): 187-199.

[29] G J Ackland, G Tichy, V Vitek, and M W Finnis, “Simple N-Body Potentials for the Noble Metals and Nickel,” Philosophical Magazine A 56, no. 6 (December 1987): 735-756.

ZrH_v4.frc

Mendelev [30]

H	H	hydrogen
Zr	Zr	zirconium

md-eam.frc

Updated pair interaction function

Zr	Zr	zirconium
Sn	Sn	tin
Cu	Cu	copper

FeNiCr_Bonny_2011.frc

EAM forcefield for alloys containing Fe, Ni, and Cr [31]

Fe	Fe	iron
Ni	Ni	nickel
Cr	Cr	cronium

AlCo_Mishin_2013.frc AlNi_Mishin_2009.frc AlTi_Mishin_2003.frc AlCu_Cai_1996.frc AlMg_Adams_1997.frc

EAM forcefields (eam/alloy format) for alloys containing Al/Co [32], Al/Ni [33], Al/Ti [34], Al/Cu [35], and Al/Mg [36].

Al	Al	aluminum
Co	Co	cobalt
Ni	Ni	nickel
Ti	Ti	titanium
Cu	Cu	copper
Mg	Mg	magnesium

---

[30] M I Mendelev and G J Ackland, “Development of an Interatomic Potential for the Simulation of Phase Transformations in Zirconium,” Philosophical Magazine A 87, no. 5 (May 2007): 349-359.

[31] G. Bonny, D. Terentyev, R.C. Pasianot, S. Poncò , and A. Bakaev, “Interatomic potential to study plasticity in stainless steels: the FeNiCr model alloy.” Modelling and simulation in materials science and engineering, 19, 085008 (2011)

[32] Purja Pun, G. P., Yamakov, V., and Mishin, Y. (2015). Interatomic potential for the ternary Ni-Al-Co system and application to atomistic modeling of the B2-L1 0 martensitic transformation. Modelling Simul. Mater. Sci. Eng., 23(6), 065006

[33] G.P. Purja Pun and Y. Mishin, “Development of an interatomic potential for the Ni-Al system,” Phil. Mag. 89, 3245 (2009).

[34] R.R. Zope and Y. Mishin, “Interatomic potentials for atomistic simulations of the Ti-Al system,” Phys. Rev. B 68, 024102 (2003)

[35] X.-Y. Liu, C.-L. Liu, and L.J. Borucki, “A new investigation of copper’s role in enhancing Al-Cu interconnect electromigration resistance from an atomistic view,” Acta Mat. 47, 3227-3231 (1999)

[36] X.-Y. Liu, P.P. Ohotnicky, J.B. Adams, C. Lane Rohrer, R.W. Hyland, Jr., “Anisotropic surface segregation in Al-Mg alloys,” Surf. Sci. 373, 357-370 (1997)

AlSiMgCuFe_MEAM.frc AuSi_MEAM.frc CH_MEAM.frc Cu_MEAM.frc FeC_MEAM.frc FeTiC_MEAM.frc Ni_MEAM.frc SiC_MEAM.frc W_MEAM.frc. . . . . . MEAM.frc

Modified EAM (MEAM) forcefields include an additional angular term for a more accurate description of metals and alloys, including Al/Si/Mg/Cu/Fe [37], Au/Si [38], C/H [39], Fe/C [40], Fe/Ti/C [41], W [42], and Si/C, Cu, and Ni from the LAMMPS website. A generic MEAM.frc is also included to be used with custom MEAM forcefield parameter sets.

AlSiMgCuFe_MEAM.frc

Al	Al	aluminum
Si	Si	silicon
Mg	Mg	magnesium
Cu	Cu	copper
Fe	Fe	iron

AuSi_MEAM.frc

Au	Au	gold
Si	Si	silver

CH_MEAM.frc

C	C	carbon
H	H	hydrogen

FeC_MEAM.frc

Fe	Fe	iron
C	C	carbon

FeTiC_MEAM.frc

Fe	Fe	iron
Ti	Ti	titanium
C	C	carbon

---

[37] B. Jelinek, S. Groh, M. Horstemeyer, J. Houze, S.G. Kim, G.J. Wagner, A. Moitra, and M.I. Baskes, “Modified embedded atom method potential for Al, Si, Mg, Cu, and Fe alloys,” Phys. Rev. B 85, 245102 (2012)

[38] J. Godet, C. Furgeaud, L. Pizzagalli, M. Demkowicz, “Uniform tensile elongation in Au-Si core-shell nanowires”, Extreme Mechanics Letters (2016)

[39] S. Nouranian, M.A. Tschopp, S.R. Gwaltney, M.I. Baskes, and M.F. Horstemeyer, “An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method,” Physical Chemistry Chemical Physics 16, 6233 (2014).

[40] L.S.I. Liyanage, S.-G. Kim, J. Houze, S. Kim, M.A. Tschopp, M.I. Baskes, and M.F. Horstemeyer, “Structural, elastic, and thermal properties of cementite (Fe13C) calculated using a modified embedded atom method,” Phys. Rev. B 89, 094102 (2014)

[41] Kim, H.-K., Jung, W.-S., and Lee, B.-J. (2009). Modified embedded-atom method interatomic potentials for the Fe-Ti-C and Fe-Ti-N ternary systems. Acta Materialia, 57(11), 3140-3147.

[42] Lee, Baskes, Kim, Cho. Phys. Rev. B, 64, 184102 (2001)

W_MEAM.frc

W	W	tungstun

SiC_MEAM.frc

Si	Si	silicon
C	C	carbon

Ni_MEAM.frc

Ni	Ni	nickel

Cu_MEAM.frc

Cu	Cu	copper

3.5 NIST Interatomic Potentials Repository

Detailed descriptions are shown in the file selection dialog. These files are distributed with consent from Chandler A. Becker, the maintainer of this repository [43], http://www.ctcms.nist.gov/potentials.

3.6 ReaxFF Forcefields

Reactive Forcefields (ReaxFF)[#30_44]_ is a family of well-established forcefields that simulate complex chemical reactions and charge transfer. It includes advanced bond terms over valence terms, shielded Coulomb, and variable charge equilibration.

AuOH.frc

ReaxFF forcefield for Au, AuO_x and water [45] from LAMMPS potentials repository

Au	Au	gold
O	O	oxygen
H	H	hydrogen

CHO.frc

The well-established ReaxFF forcefield for combustion [46] simulations from LAMMPS potentials repository

---

[43] Chandler A Becker, Francesca Tavazza, Zachary T Trautt, and Robert A Buarque de Macedo, "Considerations for Choosing and Using Force Fields and Interatomic Potentials in Materials Science and Engineering," *Current Opinion in Solid State and Materials Science* 17 (December 2013): 277-283.

[45] Keith, J. A. et al. Phys Rev B 2010, 81, 235404

[46] 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)

C	C	carbon
O	O	oxygen
H	H	hydrogen

CHON.frc

The well-established ReaxFF forcefield for nitramines (RDX/HMX/TATB/PETN) [47] from LAMMPS potentials repository

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen

HONB.frc

ReaxFF forcefield for Ammonia Borane [48] from LAMMPS potentials repository

B	B	boron
O	O	oxygen
H	H	hydrogen
N	N	nitrogen

VCHO.frc

ReaxFF forcefield for V, VOx and water [49] from LAMMPS potentials repository

V	V	vanadium
O	O	oxygen
H	H	hydrogen
C	C	carbon

ZnOH.frc

ReaxFF forcefield for Zn, ZnOx and water [50] from LAMMPS potentials repository

Zn	Zn	zinc
O	O	oxygen
H	H	hydrogen

FeCOH.frc

ReaxFF forcefield for Fe, FeOx and water [51] from LAMMPS potentials repository

---

[47] Strachan et al, Phys Rev Lett, 91, 098301 (2003)
[48] Weismiller, van Duin, Lee, Yetter, J Phys Chem A, 114, 5485-5492 (2010)
[49] Chenoweth et al, J Phys Chem C, 112, 14645-14654 (2008)
[50] Raymand, van Duin, Spangberg, Goddard and Hermansson, Surf Sci, 604, 741-752 (2010)
[51] Aryanpour, van Duin and Kubicki, J Phys Chem A, 114, 6298-6307 (2010)

V	V	vanadium
O	O	oxygen
H	H	hydrogen
C	C	carbon

CHONSFPtClNi.frc

ReaxFF forcefield for fluorinated graphene, Pt [52] from LAMMPS potentials repository

C	C	carbon
O	O	oxygen
H	H	hydrogen
N	N	nitrogen
S	S	sulfur
F	F	fluorine
Pt	Pt	platinum
Cl	Cl	chlorine
Ni	Ni	nickel

4 The MaterialsDesign Forcefield Format - FRC

The advantages of the .frc format are as follows:

- **automated atom type assignment** using the templates section of the .frc file
- **wildcards**
- **atom type equivalences** for nonbonds, bonds, angles, torsions, etc.
- **versioning**: each parameter has its own version, so updates do not remove older parameters but override them
- **includes**: a user can modify a forcefield by including the original, adding parameters and, by using version numbers, override parameters in the original

The .frc format is much more compact and makes it easy to see and edit parameters. Wildcards are the ability to specify '*' for an atom type. For example, the AUA forcefield specifies angles as C-CH2-C, where the terminal C can be almost any type of C atom, -CH3, -CH2-, -CH<, olefinic, ketone, etc. When you enumerate the permutations, it grows to be a very large list, which must be explicitly enumerated in e.g. GIBBS' potparam.dat file.

With wildcards once specify one angle as *-CH2-*, where * matches any atom. More specific angles, like an alcohol *-C-O, including completely specific ones such as H-C-O take precedence in the obvious order. This also occurs in torsions, where typically the terminal atoms do not matter: *-CH2-CH2-*

For an example of the power of including forcefield files and version numbers, look at the oplsaa+.frc file, which includes the original oplsaa.frc, extensions published elsewhere (oplsaa-extended.frc), and adds some customs additions by MaterialsDesign:

Include FF

```
!MD forcefield 1
#version oplsaa+.frc 1.0 12-Aug-2010
#define oplsaa+ default
```

---

[52] Singh, Phys Rev AB 87, 104114 (2013)

```
!Ver Ref Function Label
!—- — ———————————————— ——
1.0 1 atom_types oplsaa oplsaa-extended oplsaa+
1.0 1 equivalence oplsaa oplsaa-extended oplsaa+
1.0 1 quadratic_bond oplsaa oplsaa-extended oplsaa+
1.0 1 quadratic_angle oplsaa oplsaa-extended oplsaa+
1.0 1 torsion_opls oplsaa oplsaa-extended oplsaa+
1.0 1 wilson_out_of_plane oplsaa oplsaa-extended oplsaa+
1.0 1 nonbond(12-6) oplsaa oplsaa-extended oplsaa+
1.0 1 bond_increments oplsaa oplsaa-extended oplsaa+
1.0 1 templates oplsaa
#include oplsaa_extended.frc
```

The first section is a definition of the OPLSAA+ forcefield, listing the functional forms and the sections of the file(s) that contain the parameters. In this case the forcefield uses the ‘OPLSAA’ section (which will come from oplsaa.frc via an include in oplsaa-extended.frc) and the ‘oplsaa+’ section (which is in this file). Next it includes the entire extended OPLS forcefield.

Atom Types

```
#atom_types oplsaa+ 200


> Atom type definitions for oplsaa+
> Masses from OPLSAA publications

!Ver Ref Type Mass Element Connections Comment
!—- — —- ——— ————————————————————
! 1.0 1 CT 12.011000 C 4 sp3 aliphatic carbon

#equivalence oplsaa+ 200
@columns nonbond bond angle torsion oop bond_increment

! Equivalences
!———————————————————
!Ver Ref Type NonB Bond Angle Torsion OOP BINCR
!—- — —- —- —- —– ——- —- ——
! 1.0 1 CT CT CT CT CT CT CT

#quadratic_bond oplsaa+ 200
> E = K2 * (R - R0)^2

!Ver Ref I J R0 K2
!—- — —- —- ——- ———
! 1.0 1 CT CT 1.5290 268.0000

#quadratic_angle oplsaa+ 200
> E = K2 * (Theta - Theta0)^2
```

```
!Ver Ref I J K Theta0 K2
!—- — —- —- —- ——— ——-
! 1.0 1 CT CT CT 112.7000 58.3500

#torsion_opls oplsaa+ 200
> E = SUM(n=1,4) { [V(n)/2] * [ 1 - ((-1)^n)cos(n*Phi + Phi0(n)) ] }
> with '1-4' interactions scaled by 0.5
@units V kcal/mol
@units Phi degree

!Ver Ref I J K L V1 Phi0 V2 Phi0 V3 Phi0 V4 Phi0
!——————————————————————————————
! 1.0 1 CT CT CT CT 1.7400 0.0 -0.1570 0.0 0.2790 0.0 0.0000 0.0

#wilson_out_of_plane oplsaa+ 200
> E = K * (Chi - Chi0)^2

!Ver Ref I J K L K Chi0
!—- — —- —- —- —- ——- —-
! 1.1 4 CT CT HC HC 0.0 0.0

#nonbond(12-6) oplsaa+ 200
> E = 4.0*eps(ij) [(r0(ij)*/r(ij))**12 - (r0(ij)*/r(ij))**6]
> where r0(ij)* = sqrt((r0(i)*)*(r0(j)*))
> eps(ij) = sqrt(eps(i) * eps(j))
@combination geometric
@type r0-eps
@units Sigma Ang
@units Epsilon kcal/mol

!Ver Ref I r0 eps
!—- — —- ——— ———
! 1.0 1 CT 3.50000 0.06600

#bond_increments oplsaa+ 200

!Ver Ref I J DeltaIJ DeltaJI
!—- — —- —- ——- ——-
! 1.0 1 CT CT 0.0000 0.0000

#reference 1
Additional Materials Design OPLSAA forcefield parameters
@Author D. Rigby
@Date 12-Aug-2010
#end
```

This section adds a new atom type for sp3 aliphatic carbon, 'CT'. Each section of the file has the name of the section optionally followed by an increment to version number, 200 in this case. This increment is added to the version numbers in the section, so the practical version number of the 'CT' atom type is 1.0+200 =

201.0. Assuming that the OPLSS/AA forcefield uses version numbers less than 200, the ‘CT’ atom type would override any ‘CT’ atom types in OPLSS/AA. This allows you to take similar forcefields and let one override the other without modifying all the version numbers.

The next section defines equivalences, which simply say that when looking for the bond parameters for ‘CAh1’use ‘CA’, but when looking for bond increase parameters, use a different value for ‘CAh1’, Thus we have a new atom type that is much like sp2 aromatic carbon, but the bond increments are different.

Equivalences

```
#equivalence oplsaa
@columns nonbond bond angle torsion oop bond_increment

! Equivalences
!——————————————————
!Ver Ref Type NonB Bond Angle Torsion OOP BINCR
!—– — —– —– —– —— ——– —– ——
1.0 1 Ar Ar Ar Ar Ar Ar Ar
1.1 4 C C C C C C C
1.0 1 CA CA CA CA CA CA CA
1.1 7 CAh1 CA CA CA CA CA CAh1
```

Having a higher version overrides the previous line, and now we can use specific bond increment parameters for our ‘CAh1’ atom type.

Bond Increments

```
#bond_increments oplsaa

!Ver Ref I J DeltaIJ DeltaJI
!—– — —– —– ———– ———–
1.0 1 CA CA 0.0000 0.0000
1.1 6 CA CZ1 0.0350 -0.0350
1.0 1 CA HA -0.1150 0.1150
1.1 9 CA OH5 0.1500 -0.1500
1.1 7 CAh1 CAh2 0.1460 -0.1460
1.1 7 CAh1 HA -0.0120 0.0120
1.1 7 CAh1 NC 0.3390 -0.3390
```

The last section of the example, the bond increment section, adds the bond parameters for our new ‘CAh1’ atom type. In addition, it adds or overrides some other bond parameters.

The final section concerns templates: It is by far the most complicated section, and unfortunately due to its nature cannot be versioned or added to. It must be taken as a whole unit because it specifies which atom type to assign to an atom in a structure, and hence is ‘aware’ of all the atom types in the forcefield and the relationship between them. Hence being monolithic.

If you need to modify the template section, copy the existing template section into the top level file and define this as the location of templates in the default section. Under normal circumstance you would inherit the template section from an included forcefield file and not touch it.

These extracts illustrate some of the important features. Each section defines how a local portion of the structure maps to an atom type. Each section is for an atom type and must contain the ‘template:’ line, which gives the topology.

Templates

```
#templates oplsaa

type: ?
! anything
template: (>*)
end_type
```

As usual, ‘*’ is a wild card.

Parentheses around the template indicate that there may be other bonds to the atom that are not contemplated in the template; square brackets indicate that the template includes all bonds, and that extra bonds are not allowed. So the first template matches anything.

The ‘*’ wildcard matches any element and the surrounding parentheses allow any number of bonds.

The atom type is ‘?’ which is our shorthand for an atom for which there are no parameters. The next template is also quite simple: it matches any argon atom, regardless of whether it has bonds to it or not. If we wanted an explicit match for just argon atoms, i.e. without any bonds, we would surround the template with square brackets instead of a parenthesis.

Template for Ar

```
type: Ar
! Argon atom
      template: (>Ar)
end_type
```

For bonds we use ‘-‘ for single bonds, ‘=’ for double bonds, ‘:’ for aromatic bonds, and ‘#’ for triple bonds; ‘~’ matches any bond order, i.e. it is a wildcard.

Template for C in esters/acids

```
type:C
! Carbonyl carbon in carboxylate esters
template: (>C(-C)(-O(-C))(=O))
end_type

type:C
! Carbonyl carbon in carboxylic acids
template: (>C(=O)(-O(-H)))
end_type
```

Modifiers can narrow down the scope of wildcards: Allowed modifiers are hybridization, aromaticity, and elements:

Templates with wildcards

```
type:CA
! SP2 aromatic carbon
template:(>C(~*)(~*)(~*))
        atom_test:1
                hybridization: SP2
                aromaticity:AROMATIC
        end_test
end_type

type:CA
! This is used for aromatic carbons that fail the aromaticity test if
! the ring checker is unable to detect a ring with more than seven
! or eight sides. The NON_AROMATIC test is to eliminate the conflict
! with the above 'CA' definition.
template: [>C(-*)(:*)(:*)]
        atom_test:1
                hybridization:SP2
                aromaticity:NON_AROMATIC
        end_test
end_type

type:CAh1
! Aromatic carbon pyridine atom 2
template: (>C(:N))
end_type

type:CAh2
! Aromatic carbon pyridine atom 3
template: (>C(:C(:N)))
end_type
```

This template is quite specific for water. The square brackets both around the entire template and about the O and second H sees to that: there can be no other bonds anywhere.

Template with square brackets

```
type:HW
! TIP3P water hydrogen
template: [>H[-O[-H]]]
end_type
```

This template is less specific, but fits e.g. CO$_2$and CS$_2$. It would also fit e.g. Ar-C-Ar and other nonsensical structures.

Template with square brackets and wildcards

```
type:c2=
! Carbon in =C= (e.g. CO2, CS2)
template: [>C[˜*][˜*]]
end_type
```

This is a key issue in forcefields: they know what they do match, but not what they don't!

With wildcards they tend to match many unintended things. So in the case of Ar-C-Ar, we would assign atom types just fine and (hopefully) still not be able to run because there would be missing Ar-C bond parameters and Ar-C-Ar angle parameters. On the other hand, if we had been lazy, and defined a set of generic bond parameters for 'C-*' and angle parameters for '*-C-*' we would be off and running … garbage! It might be reasonable to have a catch-all angle term like '*-C-*' since specific hybridization of the carbon atom (sp in this case) does roughly define the angle terms. But never a bond term like 'C-*'! That is not reasonable since the bond length and strength depends on the second atom. And it is very dangerous, though the code will let you be foolish.

This brings us to more restraint use of wildcards: Here we see explicit tests that limit the power of the wildcards. The atom numbers are in the order the atoms appear in the templates, so the carbon of interest must be sp2; the two atoms other than oxygen that are bonded to it must be a C or H and an O or N. In other words this will match -C-C(=O)-OH, or H-C(=O)-OH, or -C-C(=O)-NH2 but not -C-C(=O)-C-. The modifiers for wildcards can be hybridization, which elements, and whether it is aromatic. At the moment, the code for recognizing hybridization and aromaticity is only partially complete.

Templates

```
type:c3'
! Carbonyl carbon [one polar substituent such as O,N]
! e.g. amide, acid and ester
template: (>C (˜O) (˜*) (˜*))
    atom_test:1
        hybridization:sp2
    end_test
    atom_test:3
        allowed_elements: C, H
    end_test
    atom_test:4
        allowed_elements: O, N
    end_test
end_type
```

The implementation in OPLS avoids the hybridization requirement and does not handle all cases, but goes through acids, esters, and, as shown amides:

Templates

```
type:C
! Carbonyl carbon in amides
template: (>C(-*)(=O)(-N(-*)(-*)))
        atom_test:2
                allowed_elements: C,H
        end_test
        atom_test:5
                allowed_elements: C,H
        end_test
        atom_test:6
                allowed_elements: C,H
        end_test
end_type
```

Though not shown in this example, templates can match next nearest neighbors, etc. For example, the template for a carbon attached to an azide (-N3 group) looks like this:

Templates

```
type: c4z
! Carbon, sp3, bonded to -N3 (azides)
template: (>C(-N(˜N(˜N)))(-*)(-*)(-*))
        atom_test:1
                hybridization:SP3
        end_test
end_type
```

The last section in the example is the precedence tree. An atom in a structure may match several templates, yielding different atom types. The precedence tree solves this ambiguity by providing a tree of atom types. The most specific match, i.e. the furthest from the trunk down a branch wins. The parentheses group the branches together but are admittedly rather hard to read.

Precedence tree

```
precedence:
(?
        (Ar)
        (C)
        (CA (CAh1 (CQ) (CAh6)) (CAh2 (CAh5) (CAh7) (CAh8)) (CAh3 (CAh4)) (CR)
        (CRh1)
        (CS (CAh9) (CSh1(CV)) (CSh2 (CAh0) (CVh1)) (CU) (CUh1) (CWh1 (CWh3)
        (CWh5)) (CWh2 (CWh4) (CWh6)) ) )
        (CM)
```

```
    (CO)
    (CT (CT1) (CTEX) (CTfn) (CTf4) )
    (CZ (CZ1) )
    (F)
    (H (HEX4) (HEX5) (HEX6) )
    (HC (HA (HC2)) (HC1) (HC2) (HC3) (HC4) (HC5) (HC6) )
    (He)
    (HO (HW) )
    (HS)
    (Kr)
    (N (N1) (N2) (N3))
    (NA (NAh2) (NAh3))
    (NB)
    (NBh1)
    (NBh2)
    (NBh3)
    (Ne)
    (NC)
    (NO)
    (NT)
    (NT0)
    (NT2 (NTC4) )
    (NT3)
    (NZ)
    (O)
    (O1)
    (O2)
    (O3)
    (O4)
    (OH (OH2 (OH3) ) (OH4) (OH5) (OW) )
    (ON)
    (OS (OS1) )
    (OW)
    (S)
    (SH)
    (SH1)
    (Xe)
)
end_precedence
```

Other groups such as AMBER do have some level of typing engines, but mostly the bio-organic community relies on the regularity of peptides, proteins and DNA to use systematic atom naming schemes and ‘template libraries’ to match the atom types. Thus a protein is built from peptide fragments that already have the atom names and atom types assigned by hand. Since there are only twenty some amino acids, creating the fragment library is quite feasible. Proteins from the PDB also have systematic names for the atoms, so the template libraries match the atom types with the names. These are not, however, very general solutions.