

Interface MD Usage

July 15, 2017



University of Colorado
Boulder



Hendrik Heinz
Department of Chemical and Biological
Engineering
Materials Science and Engineering Program
University of Colorado-Boulder, CO, USA



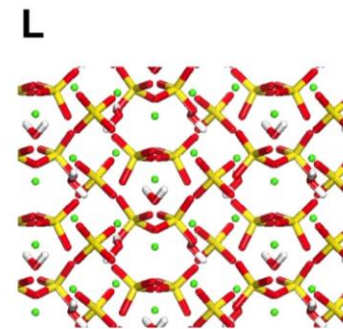
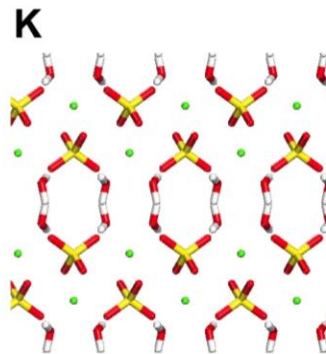
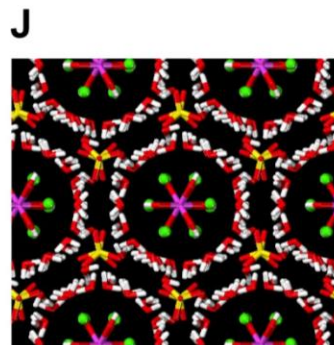
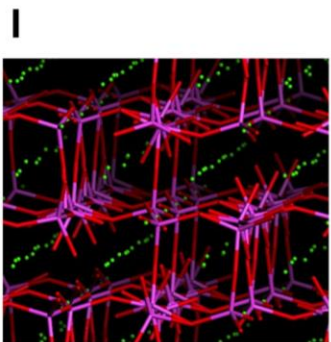
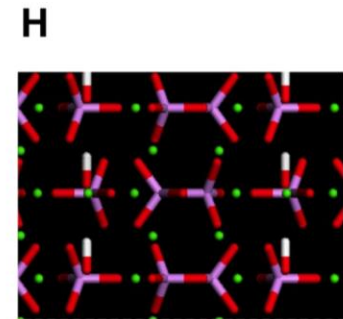
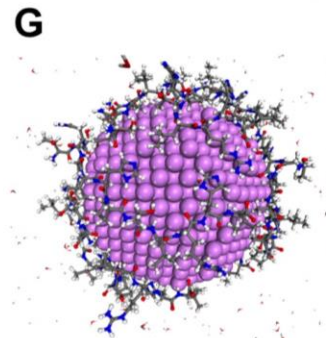
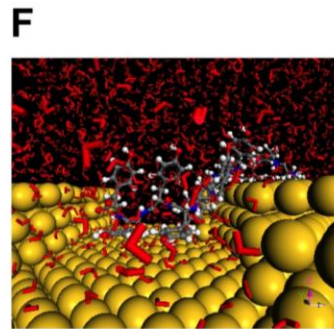
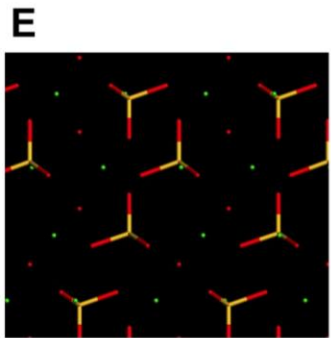
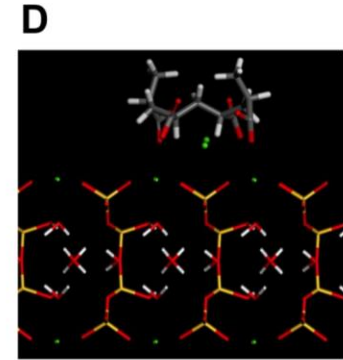
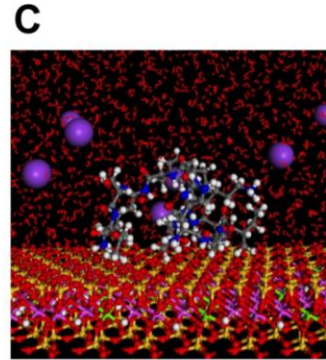
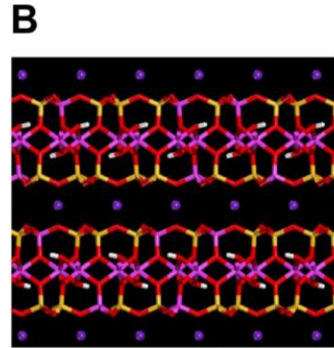
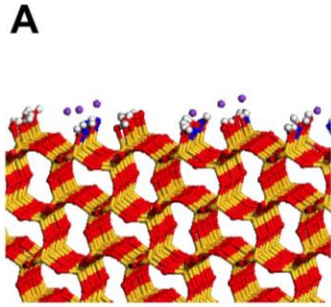
IFF - List of Compounds Currently Included

- **Layered silicates:** mica, different montmorillonites, pyrophyllite, kaolinite including surfaces of different CEC and cation distributions according to NMR data
- **Fcc metals:** Ag, Al, Au, Cu, Ni, Pb, Pd, Pt, including {111}, {100}, and {110} surfaces
- **Silica:** bulk minerals (quartz, cristobalite) as well as surfaces of different degree of ionization for specific pH values and particle sizes (comprehensive database)
- **Hydroxyapatite:** bulk mineral, different cleavage planes, nanorods for various pH
- **Cement minerals/LDH:** tricalcium silicate, tricalcium aluminate, ettringite, monosulfate (hydrocalumite), tobermorite 11 Å, tobermorite 14 Å, C-S-H, including different cleavage planes
- **Calcium sulfates:** calcium sulfate hemihydrate and gypsum, including different cleavage planes
- **Poly(ethylene oxide):** crystal and polymer chain including gauche effect and approximate solubility (radius of gyration) in water

(Extensible to similar/other compounds)



Compounds Included: Clays, FCC Metals, Silica, Apatites, Cement Minerals





Features and Capabilities

- Accurate parameters for inorganic compounds
 - Reduction in >500% deviation in interfacial properties from experiment in earlier models to <10%
- Enable simulations of multiple materials classes (inorganic, organic, biomolecules)
 - Fully compatible with biomolecular and materials oriented force fields (energy expressions)
 - Applicable to biointerfaces, metals, ceramics, polymers, construction materials
- Emphasis on chemically meaningful atomic charges and van-der-Waals parameters with thorough validation by measured atomic-scale and surface properties
- ***Open to parameterization of further compounds by users*** and integration in community simulation software (CHARMM, GROMACS, BIOVIA, Tripos, ...)
- Limitations and further developments: reactions, polarizability, more compounds (graphene, organic semiconductors, quantum dots ..)



Use in Materials Studio

Neat IFF compounds

Supported force fields: CVFF-IFF, PCFF-IFF

- 1) Load unit cells or surface models from surface model database
 - Customize supercells, nanostructures, or surface chemistry, maintaining IFF atom types and charging schemes

Turn off automatic typing and automatic charge calculation. If overridden, the reliability of the simulation is voided

- 2) Run MD/MC simulation using Discover (.frc file) or Forcite (.off file)

For multiphase systems including water, organic molecules, or biomolecules

- 3) Build models of water, surfactant, drug, protein etc using Materials Studio visualizer
- 4) Assign automatically – for these components only – atom types and charges according to the default cvff-interface or pcff-interface rules
- 5) Build combined simulation input of inorganic/organic structure (e.g. copy-paste) using IFF models for the inorganic phase

Turn off automatic typing and automatic charge calculation

- 6) Run MD/MC simulation using Discover or Forcite



Use in LAMMPS

Supported force fields: CVFF-IFF, PCFF-IFF, CHARMM-IFF

- 1) Prepare input in Materials Studio, export Insight .car/.mdf files
- 2) Run msi2Imp tool in the command line, supplying the location of the respective cvff_interface.frc / pcff_interface.frc file

Alternative: Prepare LAMMPS input file using other visualizers/builders (e.g. convert from CHARMM using charmm2Imp). Verify correct atom types and charges.

- 3) Run LAMMPS using the .lammps05 file and standard LAMMPS input scripts

Observe settings of bonded & nonbonded parameters in LAMMPS input scripts for cvff, pcff, or charmm (use the respective definition)

CVFF (no cross no morse)

```
kspace_style      ppm 1.0e-6
pair_style        lj/cut/coul/long 12.0 8.0

bond_style        harmonic
angle_style       harmonic
dihedral_style    harmonic
improper_style    cvff
```

PCFF

```
kspace_style      ppm 1.0e-6
pair_style        lj/class2/coul/long 12.0

bond_style        class2
angle_style       class2
dihedral_style    class2
improper_style    class2
```

CHARMM

```
kspace_style      ppm 1.0e-6
pair_style        lj/charmm/coul/long 12.0 8.0
pair_modify       mix arithmetic

bond_style        harmonic
angle_style       charmm
dihedral_style    charmm
improper_style    harmonic
```



Use in NAMD

Supported force fields: CHARMM-IFF

1) Prepare input in Materials Studio, export Insight .car/.mdf files

For all non-IFF compounds, use CHARMM atom types, charges, and bond connectivity (topology)

2) Use msi2namd, including an .frc file for the IFF compounds, to convert to .pdb/.psf in a single command

3) Run NAMD using standard NAMD input scripts

Alternative: Prepare .pdb/.psf files using other means (CHARMM topology file, psfgen, CHARMM-GUI). Check correct atom types and charges, bond connectivity, as well as suitable residue names for IFF compounds.

An implementation of IFF in CHARMM-GUI is in progress.



Use in GROMACS

Supported force fields: CHARMM-UFF; GROMACS/GROMOS and OPLS-AA manually

1) CHARMM-UFF parameters for compounds of interest must be manually inserted into the parameter files for GROMACS.

Attention for 12-6 Lennard-Jones parameters:

1) ϵ (GROMACS) = $4.184 \cdot \epsilon$ (CHARMM) due to units of kJ/mol, not kcal/mol

2) σ (GROMACS) = σ (CHARMM) / $2^{1/6}$ and given in nm, not in Å

Attention for bond and angle parameters:

GROMACS uses pre-factor $\frac{1}{2}$ for harmonic potentials, i.e., k (GRO) = $2 k$ (CHA)

2) The structural models must be built with desired coordinates. Then, UFF-specific and GROMACS-specific atom types and charges need to be assigned in a manual or semi-automated way. All covalent bonds for UFF components must be specified (can be verified with supplied surface models in the UFF database).

3) Run MD simulation with GROMACS

Caution when using GROMACS with OPLS-AA for systems with 1,4 covalent bonds (clays, silica, etc). The specific 1,4 nonbond exclusions of OPLS-AA may require modifications of CHARMM-UFF parameters.



Use with OPLS-AA

Supported force fields: OPLS-IFF, manually

For metals, apatites, sulfates, and several cement minerals, the 12-6 LJ and bonded parameters can be imported into OPLS-AA and directly used.

- 1) CHARMM-IFF (or OPLS-IFF) parameters for compounds of interest must be manually added to the parameter files for OPLS-AA.
- 2) Structural models can be built using the IFF-specific and OPLS-AA specific atom types, charges, and specifying all covalent bonds (verifiable using the supplied surface models in the IFF database).
- 3) Run MD simulation using a suitable program (GROMACS, Desmond, etc).

Note: For some compounds with 1,4 bonded interactions, the OPLS-AA force field requires specific parameters. See, e.g., Dalton Trans. 2014, 43, 10602, for tricalcium aluminate. Modifications of the CHARMM parameters may be necessary.



Use with AMBER, DL-POLY, Other Programs

Supported force fields: AMBER, others

1) Include the IFF parameters for compounds of interest manually in the parameter files for AMBER, DL-POLY, and other desired programs using the correct units.

2) Build the structural models with desired initial coordinates. Then, assign the IFF-specific and AMBER-specific force field (atom) types and charges in a manual or semi-automated way. Specify correctly all covalent bonds for IFF components (use the supplied surface models in the database to verify).

Note: (1) IFF follows standard combination rules and rules for scaling of nonbond interactions between 1,4 bonded atoms for a given parent force field (CHARMM, AMBER, PCFF etc). Therefore, for some compounds with 1,4 bonded interactions, CHARMM parameters cannot be directly applied in OPLS-AA and AMBER. Small modifications may be necessary, e.g., see Dalton Trans. 2014, 43, 10602, for tricalcium aluminate. (2) Do not override atom types and atomic charges as defined in IFF for all IFF compounds at any time during the simulation (e.g. by hidden automation upon start of MD simulations).

3) Run MD/MC simulation using AMBER, DL-POLY, and other simulation programs.

Efforts towards automated, GUI-supported input conversion are in progress.