MedeA ReaxFF

Simulate Chemical Reactions with High Resolution at Real Conditions

At-a-Glance

With *MedeA ReaxFF* computationally investigate chemical reactions in solid, liquids, and gases at the atomic scale, for spatial domains on the order of several nanometers and time ranges up to several nanoseconds. On demand the underlying molecular dynamics simulations explicitly consider temperature, pressure, and other extrinsic properties, such as applied electric fields.

Key Benefits

- **Applicability** - Employ *MedeA ReaxFF* to predict structural and mechanical properties of materials and energetics of chemical processes and reactions in catalysis, batteries, fabrication of semiconducting devices, and many more
- **Coverage** - *MedeA ReaxFF* provides parameters sets for about 50% of the chemical elements
- **Productivity** - Fully integrated in the *MedeA Environment* to benefit from the versatile builders, flowchart and high-throughput capabilities, and smart post-processing of results

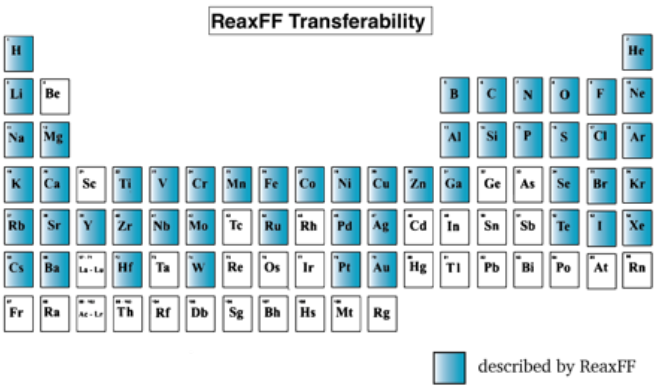

Figure 1: Coverage of ReaxFF parameters set in MedeA

Key Features

- *MedeA ReaxFF* fully utilizes the powerful molecular dynamics engine *LAMMPS*[1], the world's leading molecular dynamics code for materials science
- *MedeA ReaxFF* is based on the well established Reactive Force Field formalism[2] which is widely used by academic and industrial research and development institutions
- *MedeA ReaxFF* accurately describes chemically reactive systems including formation and breaking of any chemical bonds (metallic, covalent, ionic, and electrostatic bonds)
- The *MedeA ReaxFF* repository currently encompasses about **40** parameter sets to describe various materials classes such as
  - organic compounds, proteins, and polymers
  - fuels, explosives, propellants, and gases under very reactive conditions
  - metals and alloys
  - clays, zeolites, and other minerals

  and combinations thereof
- *MedeA ReaxFF* is continuously extended and any additional parameter set that was published or custom generated can be easily imported

Required Modules

- *MedeA Environment*
- *MedeA ReaxFF*

Related Modules

- *MedeA Deposition*
- *MedeA EAM*
- *MedeA COMB3*

[1] S.J. Plimpton, "Fast Parallel Algorithms for Short-Range Molecular Dynamics", *J. Comp. Phys.* **117**, 1 (1995) DOI

[2] A.C.T. van Duin, *et al.*, *J. Phys. Chem. A* 105, 9396 (2001)

Recommended Modules

- *MedeA VASP 5*
- *MedeA Diffusion*
- *MedeA Viscosity*
- *MedeA Thermal Conductivity*
- *MedeA Docking*
- *MedeA Amorphous Materials Builder*
- *MedeA MT*
- *MedeA HT-Launchpad*

Find Out More

Contact Materials Design to see *MedeA ReaxFF* in action in the following tutorials:

- Running ReaxFF in MedeA
- H_2O Dissociation on ZnO Surface with ReaxFF
- Deposition of O_2 on Si Surface with reactive forcefields

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