MedeA Forcefield

While forcefield-based calculations can be really powerful, forcefields themselves can be really painful. No longer! Our Forcefield module provides state-of-the-art forcefields along with the support and tools that you need to make them work for you, rather than the other way around.

Key Benefits of MedeA Forcefield:

- Leading forcefields from many areas, assembled and checked by experts
- Automatic assignment of atom types and charges
- Customizable forcefields
  - Safely add and change parameters when needed
  - Changes are kept separate and not overwritten by updates
  - Version tracking to keep all modifications accessible for evaluation and comparison
  - Possibility to work with Materials Design’s forcefield experts in the development of customized solutions
- Materials Design’s experts provide industrial-level support of forcefields shipped with MedeA

Forcefields Included:

- Forcefields for organic molecules, polymers, carbon nanotubes, etc.
  - OPLS-AA
  - PCFF
  - Enhanced PCFF with refined nonbond parameters
  - COMPASS (published part)
  - CFF91 & CFF93
  - CVFF
  - AUA-4 (Anisotropic United Atom, Gibbs only)
- Forcefields for semiconductors
  - Stillinger-Weber
  - Tersoff
- Forcefields for inorganic compounds: zeolites, perovskites, phosphates, glasses, etc.
  - CVFF-AUG
  - Inorganic

E = A e^{-r/r_c} - \frac{C}{r^6} \quad \text{with} \quad r < r_c

\frac{E}{4} = \begin{pmatrix} \phi \theta \\ \theta \phi \end{pmatrix} \begin{pmatrix} \phi \\ \theta \end{pmatrix}

E = D \left(1 - e^{-r/r_c}\right)^2

\phi = \psi \sin(\theta) \cos(\phi) + \psi \sin(\theta) \sin(\phi) + \psi \cos(\theta)

E = \sum_i \left( F_i(\bar{r}_i) + \frac{1}{2} \sum_{j<i} \phi_{ij}(\bar{r}_{ij}) \right)

E = C \left[ 1 - B (-1)^n \cos(n \phi) \right]

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