SI2-SSE: Enabling Chemical Accuracy in Computer Simulations: An Integrated Software Platform for Many-Body Molecular Dynamics

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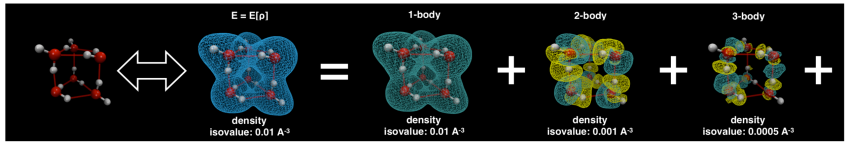
Goal

Make MB-MD methodology widely available to a broad scientific community via user-friendly and efficient software tools

Many-body molecular dynamics

- No recourse to empirical parameters
- Potential energy functions entirely derived from correlated electronic structure data
- Enables predictive molecular simulations across different phases

$$E_N = \sum_i^N V^{1B}(i) \quad \text{1-body}$$
$$+ \sum_{i<j}^N V^{2B}(i,j) \quad \text{2-body}$$
$$+ \sum_{i<j<k}^N V^{3B}(i,j,k) \quad \text{3-body}$$
$$+ \ldots$$
$$+ V^{NB}(1,\ldots,N) \quad \text{N-body}$$



MB-fit

- Workflow system for machine learning of many-body potential energy functions
- Python based with Jupyter notebooks for user documentation
- Centralized PostgreSQL data storage

Broader Impacts

- Training of postdocs, graduate and undergraduate students, high school interns in computational research and software engineering
- Software tools to empower new applications ranging from chemistry to material discovery

MBX

- C++ library for MB-MD simulations
- Periodic boundary conditions with PME for electrostatics and dispersion
- OpenMP parallel
- User-friendly API for integration with simulation codes
- Interface to i-PI and PLUMED