Open questions and needs from hard and soft materials: Ab initio methods

Shared metadata and data formats for
Big-Data Driven Materials Science

July 9, Berlin

Goals

- Discuss open questions
- New areas to cover
- Improvements and extensions to existing metadata
- Feed ideas and topics to tomorrow's working groups
- Protocol on how to proceed

Topics covered in the 2016 workshop

- Metadata for code-independent format
- Common energy zero for total energies
- Electronic and vibrational properties of solids
- Compact representation of scalar fields: density, wavefunction, xc potentials, etc
- Quantities related to excited-state calculations

Metadata for code-independent format

Driving forces for the NOMAD Meta Info evolution:

- NOMAD Laboratory (analytics, encyclopedia, etc)
- NOMAD parser development

Metadata for code-independent format

Driving forces for the NOMAD Meta Info evolution:

- NOMAD Laboratory (analytics, encyclopedia, etc)
- NOMAD parser development

Challenges

- New metrics: quality, effectiveness, performance
- Framing the Meta Info into a proper ontology
- Interoperability
- Coordinate the Meta Info development among all stakeholders

Selected topics

Ab initio

- Common energy zero for total energies
- Compact representation of scalar fields
- Exchange-correlation
- Basis sets

Common to Ab initio and Molecular Mechanics

- Workflows and processes
- Provenance: tracking and identification
- Equivalence and similarity

Common energy zero for total energies

Strategy

- Define relative energies
- Reference: isolated atoms and simple bulk systems
- Fully converged calculation: one value per physical model (xc functional, pseudopotential, etc)
- Alternative: use the same numerical setting as original calculation

Compact representation of scalar fields

How to compare scalar fields (densities, potentials, etc) obtained with different codes using different basis sets?

Proposed solution:

- Conversion to a universal basis set
- Some promising candidates:
  - Guassian basis function
  - Numerical atomic orbitals

Compact representation of one-particle wavefunctions and scalar fields obtained from electronic-structure calculations, Sergey V. Levchenko, Matthias Scheffler, Comput. Phys. Comm. **237**, 42-46 (2019)

Basis sets

- Basis set families: atom-centered or cell-dependent
- NOMAD Meta Info mostly complete for atom-centered
- Very incomplete for cell-dependent: nothing about finite differences/elements, wavelets, etc

Exchange-correlation functionals

- Essential ingredient for reproducibility
- Specification of xc functionals is increasing in complexity (combination of functionals, parameter tweaking)
- Number of functionals is continuously increasing (approx. 500)
- Need a standardized parameter specification
- Need to distinguish between functional forms and particular parameterizations