MM 59: Computational Materials Modelling - Potentials

Time: Thursday 15:45–17:15   Location: IFW A

MM 59.1 Thu 15:45 IFW A
A platform for the validation of interatomic potentials —
●Yury Lysogorskiy, Thomas Hammerschmidt, and Ralf Drautz
— AMS, ICAMS, Ruhr University Bochum, Bochum, Germany

Interatomic potentials (IPs) are widely used in computational mate-
rials science, in particular for simulations that are too computation-
ally expensive for density functional theory (DFT). A large number
of IPs is available for a wide range of chemical elements and their
mixtures. Most IPs have a limited application range and often there
is very limited information available regarding their performance for
specific simulations. We performed extensive tests for the majority of
the available potentials from the OpenKIM and NIST repositories as
well as from other sources. In this talk we present the online platform
atomistictools.org for the validation of IPs. The platform offers effi-
cient visualization of various tests and ranking of the IPs. Predictions
of the IPs are compared to reference data (DFT and experiment, if
available). The platform further provides direct access to the tests,
reference data and protocols in order to that potential developers can
integrate this into their workflow for parameterizing novel potentials.

MM 59.2 Thu 16:00 IFW A
**Machine-learned density-functional tight-binding: Enabling
high-quality electronic structure calculations on systems too
large for DFT** — ●Simon Anniés, Chiara Panosetti, Christoph
Scheurer, and Karsten Reuter — Technical University Munich

Density-Functional Theory (DFT) has been one of the go-to methods
for electronic structure calculations for several decades. Nevertheless,
inherent scaling properties and/or large prefactors for linear-scaling
implementations still limit its usability for larger systems or extensive
sampling.
   Density-Functional Tight-Binding (DFTB), a semi-empirical ap-
proximation to DFT, is an alternative that - as opposed to forcefields
- retains access to electronic structure properties while providing a
speed-up of roughly three orders of magnitude. The trade-off is a
two-part parametrization process. The numerical parameters of the
electronic part are optimized by comparing with DFT bandstructures,
the repulsion potential by forcematching against representative train-
ing sets from high-level electronic structure methods.
   In our work, we apply a machine learning approach, making use
of Gaussian Process Regression (GPR), in order to greatly increase
the adaptability of the repulsion potential. By embracing a purely
data-driven methodology, this overcomes the limitations of previously
employed rigid functional forms. We demonstrate the superior trans-
ferability of this approach in the application to lithium-intercalated
graphite as prevalent anode material of commercial lithium-ion bat-
teries.

MM 59.3 Thu 16:15 IFW A
**Machine Learning Augmented Density Functional Tight
Binding Theory** — ●Adam McSloy[1], Benjamin Hourahine[2],
David Yaron[3], and Reinhard J. Maurer[1] — [1]Department of
Chemistry, University of Warwick — [2]Department of Physics, Uni-
versity of Strathclyde — [3]Department of Chemistry, Carnegie Mellon
University

Density functional tight binding theory (DFTB) is a cost-effective elec-
tronic structure method which excels at reaching the size and time
scales normally off limits to Density Functional Theory and other elec-
tronic structure methods. However, the derivation of parameter sets
for systems beyond simple semiconductors and organic molecules is a
non-trivial task. Here, we present a deep machine learning framework
to construct DFTB parameter sets and apply it to construct a new
parameter set for hybrid organic-metallic materials. Furthermore, we
show that machine learning offers a way to extend the DFTB method
beyond the two-centre approximation, which enables a more accurate
treatment of reactive chemistry and non-equilibrium dynamics.

MM 59.4 Thu 16:30 IFW A
**Towards transferable parametrization of Density-Functional
Tight-Binding with machine learning** — ●Leonardo Medrano
Sandonas, Martin Stöhr, and Alexandre Tkatchenko —
Physics and Materials Science Research Unit, University of Luxem-

bourg, Luxembourg.

Machine learning (ML) has been proven to be an extremely valuable
tool for simulations with ab initio accuracy at the computational cost
between classical interatomic potentials and density-functional approx-
imations. Similar efficiency can only be achieved by semi-empirical
methods, such as density-functional tight-binding (DFTB). One of the
limiting factors in terms of the accuracy and transferability of DFTB
parametrizations is the so-called repulsive potential, which plays a con-
siderable role for the prediction of energetic, structural, and dynamical
properties. Few attempts of using ML-techniques to address this issue
have been proposed recently [1] but, up to now, evidence of trans-
ferability and scalability is still scarce. Using the QM7-X database
of small organic molecules, we demonstrate that the DFTB repulsive
energy can be effectively learned by means of ML-approaches includ-
ing neural networks and kernel ridge regression. We further show how
the resulting DFTB+ML model can also be used for more complex
systems like molecular dimers and crystals, and modeling techniques
like (global) structure search or vibrational analysis. DFTB+ML thus
opens a route to the simultaneous access to reliable electronic and
structural/dynamical properties of diverse molecular systems. [1] J. J.
Kranz et al., J. Chem. Theory Comput., 14, 2341-2352, (2018).

MM 59.5 Thu 16:45 IFW A
Anharmonic phonons at elevated temperatures in Al —
●Michael Leitner[1] and Albert Glensk[2,3] — [1]Technische Univer-
sität München, 85748 Garching, Germany — [2]Ecole Polytechnique
Federale de Lausanne, 1015 Lausanne, Switzerland — [3]Max-Planck-
Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

The importance of anharmonicity for describing fundamental materi-
als properties, starting from finite heat conductivity due to phonon-
phonon scattering, can hardly be overemphasized. For crystalline mat-
ter, the principal microscopic gauge is constituted by the broadening
in energy of the phonon dispersions, corresponding to q-dependent
phonon lifetimes.
   Here the case of elemental Al at temperatures up to the melting
point will be considered. Experimental data obtained by inelastic neu-
tron scattering will be compared to calculations of q-dependent line
broadenings on the basis of density-functional theory. The agreement
with spectra computed by ab initio molecular dynamics is satisfactory,
while the standard approach of perturbation theory gives significant
discrepancies. Finally, an analysis of the atomic interaction constants
will show how numerically efficient phenomenological potentials can be
constructed that allow to compute anharmonic properties beyond the
limitations of perturbation theory at very small computational effort.
   A. Glensk et al., to be published in Phys. Rev. Lett. (2019)

MM 59.6 Thu 17:00 IFW A
**Comparative Study of Interatomic Potentials for Atomistic
Simulations of Sintering of α-Alumina** — ●Arun Prakash,
Shyamal Roy, and Stefan Sandfeld — Micromechanical Materi-
als Modelling (MiMM), Institute of Mechanics and Fluid Dynamics,
TU Bergakademie Freiberg

Crystalline alumina (α-alumina) with a corundum structure exhibits
excellent material properties and is usually processed via sintering. At
the nanoscale, sintering and the properties of the sintered material
are often determined by atomic scale processes. Atomistic simulations
are ideally suited to study and gain valuable insights into such funda-
mental processes, but their accuracy is, however, determined by the
interatomic potential used.
   In this work, we perform a systematic study of different interatomic
potentials for the sintering of α-Al_2O_3 via atomistic simulations. The
compared potentials are: Vashishta, Buckingham/Matsui type, Born-
Mayer-Huggins type and Charge Transfer Ionic + EAM (CTI+EAM).
We first compare fundamental properties like e.g. surface energies,
elastic constants etc. via molecular statics, and then simulate sinter-
ing of thin slab like structures via molecular dynamics. We analyze
the simulations in terms of both global quantities and local mecha-
nisms. The differences in the sintering simulations are correlated to
the fundamental properties of the individual potentials. Finally, we
discuss the consequences of the usage of such potentials for atomistic
simulations