INSTITUTE FOR COMPUTATIONAL PHYSICS

Universität Stuttgart

Einladung zum ICP-Kolloquium

via zoom https://zoom.us/j/93720564810?pwd=QXcvZ0Foa1RmU3RKRW5kZE5YVGdFZz09
Meeting ID: 937 2056 4810, Passcode: 467207

Auskunft: Dr. Alexander Schlaich, Tel: 0711-685 63607

Gábor Csányi
Engineering Laboratory, University of Cambridge

hält am

Donnerstag, 14. Januar 2021, 16:00 Uhr

einen Vortrag über das Thema:

"Machine learned force fields: status and challenges"

Abstract:

I will make the somewhat bold claim that over the past 10 years, a new computational task has been defined and solved for extended material systems: this is the systematic analytic fitting of the Born-Oppenheimer potential energy surface as a function of nuclear coordinates under the assumption of medium-range interactions, out to 5-10 Å. The resulting potentials are reactive, many-body, reach accuracies of a few meV/atom, with costs that are on the order of 1-10 ms/atom. Important challenges remain: treatment of long range interactions in a nontrivial way, e.g. environment dependent multipoles, charge transfer, magnetism. Time is ripe for a "shakedown" of the details among various approaches (neural networks, kernels, polynomials), and more standard protocols of putting together the training data. Tradeoffs between system- (or even project-) specific fits vs. more general potentials will be ongoing. I am particularly concerned with the amount physics and chemistry that we impute into these approximations, and they can be used to help "extrapolate" correctly into regions of configuration space far from those in the data set.

Interessenten sind herzlich eingeladen.

Prof. Dr. C. Holm
Apl. Prof. Dr. R. Hilfer
Apl. Prof. Dr. M. Fyta