Julius-Maximilians-
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Kolloquium der Physikalischen und Theoretischen Chemie

Dienstag, 07.07.2015 **Hörsaal D, Chemiezentralgebäude, 17:15 Uhr**

Sprecher: **Judith Rommel**
(Cambridge, UK)

Titel: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters

Abstract:

Increasingly, chemical productions and industrial applications use computational models and predictions based on large data sets to design new materials. These include highly efficient catalysts, new energy sources, or materials for energy storage. Embedded atom methods,[1, 2] modified and enhanced over the last decades, are popular models to describe structural, mechanical, and thermal properties of large metallic systems with several thousand atoms due to their scaling in performance compared to first-principles calculations. In this presentation, I will address the following questions:

- Where do several of these models break down, e.g., D.G. Truhlar's Embedded Atom Method (EAM) and M.I. Baskes' Modified EAM for CH_4 on Ni(100)?
- How can existing models be improved?
- How can we choose a good model?

I will present alternative ways to explore and assess the quality of models by looking at the analysis of Gaussian process visual response surfaces to find parameters as well as the uncertainty of parameter set estimations. In future, similar approaches will increase the credibility of computer simulations and ease the judgement of simulation models and methods. Ultimately, modelling of materials will be moved to a level where a careful reliability check of the simulations goes hand in hand with the design of new optimized catalysts and functional materials.

References
1 M.S. Daw and M.I. Baskes. Phys. Rev. Lett. 50 (17), 1285 (1983).
2 M.S. Daw and M.I. Baskes. Phys. Rev. B 29 (12), 6443 (1984).

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