IAP Seminar

Christopher Heard

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Tuesday, 14th June 2022, 16:00 s.t.
TU Wien, Institut für Angewandte Physik, E134
1040 Wien, Wiedner Hauptstraße 8-10
Yellow Tower „B“, 5th floor, SEM.R. DB gelb 05 B

The seminar will be also held as a Zoom Meeting
https://tuwien.zoom.us/j/96269599040?pwd=NG56a0pncXp0WjhjT2V2T1hLUEJGZz09

Towards Operando Modelling in Zeolites: Solvation, Encapsulation, Diffusion

Zeolites represent an important class of environmentally friendly and commercially available solid catalysts and are produced at the Mega-tonne scale. Optimal utilization requires an atomistic understanding of framework structure, as well as both reactive and non-reactive processes occurring within the micropore. However, intercage diffusion, cluster agglomeration and redispersion are complex processes which generally occur on timescales too long for traditional computational modelling methods. We tackle this problem *via* the development of flexible, reactive neural network potentials with density functional theory accuracy, which dramatically extend sampling quality, and allow for investigations of complex, reactive environments in zeolites.

In this talk I will discuss recent developments from our group towards *operando* modelling of zeolites, including the training of multi-elemental, reactive machine learning potentials, and their applications in:

- *In silico* screening of siliceous frameworks
- Incorporation, diffusion and reactions of water within micropores
- Stabilization and migration of zeolite-encapsulated sub-nanoscale Pt clusters

All interested colleagues are welcome to this seminar lecture
(45 min. presentation followed by discussion).

Friedrich Aumayr
(LVA-Leiter)

Gareth Parkinson
(Seminar Chair)