

Thijs J.H. Vlugt

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Monday, 11th December 2023, 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/69482846795?pwd=TENsTWVIMkEyemd3Y2tjellsYVQrUT09>

Thermodynamics and transport properties of systems containing water, hydrogen, and salts

Understanding the thermodynamics and transport properties of systems containing water, hydrogen, and salts is important for the energy transition, e.g. for underground hydrogen storage, electrochemical compression of hydrogen, and alkaline electrolysis. In my presentation, I will discuss how molecular simulation can be used to model these systems and what main limitations are. Examples are: controlling the water content in high-pressure hydrogen, solubility and diffusion of hydrogen in potassium hydroxide solutions, and the recent 2-surfaces approach, in which one potential energy surface is used to model intermolecular interactions, and another one is used to compute free energies.

Prof. Dr. Thijs J.H. Vlugt is a full Professor at Process and Energy Department at TU Delft and the Chair of Engineering Thermodynamics. He received his PhD degree at the University of Amsterdam with R. Krishna and Berend Smit as thesis advisors. After postdoctoral research in Mainz (Germany) and Leiden (The Netherlands), he was appointed as an assistant professor at Utrecht University in The Netherlands. In 2007 he moved to Delft University of Technology, first as Associate Professor and later as full professor.

Prof. Vlugt mainly works on the design of process fluids and other materials enabling efficient chemical processes and energy technology. His group further focus on interfacial behavior and transport at the molecular/nanoscale. He uses Molecular Thermodynamics and Molecular Simulations as basis of his research for many practical fields such as CO₂ capture, hydrogen storage and energy transition.

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

Friedrich Aumayr
(LVA-Leiter)

Markus Valtiner
(Seminar Chair)