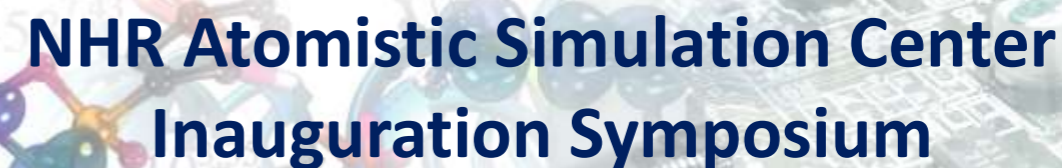




NHR



NHR Atomistic Simulation Center Inauguration Symposium

Full Program and Registration: <https://tiny.cc/ASC-NHR-2021/>

Atomistic Simulation Center

Paderborn – Erlangen – Berlin
Inauguration Symposium

Online

26 – 27 October 2021 | 14:00 – 18:40

Invited Speakers

Ralf Drautz (Ruhr-Universität Bochum)

Holger Gohlke (Heinrich-Heine-Universität Düsseldorf)

Frauke Gräter (Heidelberger Institut für Theoretische Studien)

Bettina Keller (Freie Universität Berlin)

Ulrich Kleinekathöfer (Jacobs University Bremen)

Christian Ochsenfeld (Ludwig-Maximilians-Universität München)

Peter Saalfrank (Universität Potsdam)

Full Program and Registration:

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Tue 26 October 2021

14:00 – 14:45 **Challenges in Atomistic Simulations through National High-Performance Computer Centers (NHR)**
G. Wellein (FAU), P. Imhof (FAU)

15:00 – 16:20 **Materials Science at the Atomic Scale**
R. Drautz (RUB), E. Bitzek (FAU), G. Schmidt (PC²)

16:40 – 18:40 **Modelling Soft Matter at the Atomic Scale**
F. Gräter (HITS), F. Höfling (ZIB), A. S. Smith (FAU),
B. Keller (FUB)

Wed 27 October 2021

14:00 – 15:20 **Life Sciences at the Atomic Scale**
U. Kleinekathöfer (JUB), H. Gohlke (HHU)

15:40 – 17:40 **Novel Approaches in Quantum Chemistry**
P. Saalfrank (UP), Ch. Ochsenfeld (LMU),
Th. Kühne (PC²), A. Görling (FAU)

18:00 – 18:40 **Technical and Algorithmic Challenges in High-Performance Computing**
Ch. Pleschl (PC²)

