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To all members of the
Faculty of Physics

Vienna, 16 May 2025

Invitation to the public defense of the doctoral thesis

"Machine Learning for Small Polaron Modeling: Stability, Transport, and Defect Interactions"

by

Viktor Christian Birschitzky

Friday, 23 May 2025, 12:00 a.m.
Ernst-Mach-Lecture Hall, 2nd floor, Boltzmanngasse 5, 1090 Vienna

Or via Zoom:
https://univienna.zoom.us/j/61065708300?pwd=5YG9akWfsB1Cahh1aunfdZ1OSZQIk7.1

Meeting ID: 610 6570 8300
Passcode: 418037

Small polarons -- localized charge carriers coupled to lattice distortions -- play a key role in determining transport properties, defect chemistry, and surface reactivity in oxide materials. However, their local character and dynamic behavior pose major challenges for first-principles modeling, especially due to the large configurational space of defect-polaron arrangements and the difficulty of capturing hopping dynamics. This dissertation explores how machine learning (ML) can overcome these challenges to enable accurate and efficient modeling of small polarons in complex oxide environments. ML models trained on DFT data predict stable configurations in Nb-doped $SrTiO_3$ and TiO_2, revealing both known and novel polaron patterns and clarifying experimental observations. Message-passing neural networks are further used to model polaron hopping in MgO and TiO_2, capturing mobilities, activation barriers, and polaron defect correlation in long-timescale simulations. These results demonstrate that ML can bridge the gap between computational efficiency and physical accuracy in polaron modeling, extending the applicability of ML-based potential energy surfaces to localized charge carriers.

Defense committee:
Ralf Drautz, Ruhr Universität Bochum, DE (reviewer)
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