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To all members of the
Faculty of Physics

Vienna, 06 June 2025

Invitation to the public defense of the doctoral thesis

"Machine-Learned Anharmonic Phonons and Their Impact on Electron-Phonon Coupling"

by

Luigi Ranalli

Thursday, 12 June 2025, 16:00 p.m.
PC-Seminarroom 1, OG01, Kolingasse 14-16, 1090 Vienna

Phonon anharmonicity and quantum fluctuations are often neglected in ab initio simulations due to their computational complexity. In this thesis, a novel computational workflow is developed by combining machine learning force fields (MLFF) with the stochastic self-consistent harmonic approximation (SSCHA), enabling accurate modeling of phonon anharmonicity and quantum dynamics.
Our methodology provides temperature-dependent phonon dispersions for \ce{KTaO3} and \ce{SrTiO3} in the quantum paraelectric regime, and facilitates the inclusion of anharmonic effects in electron-phonon coupling calculations. We compute the electron mobility in these materials using the Boltzmann transport equation, accounting for lattice disorder and bandstructure renormalization through the ZG method. The observed discrepancies with experimental data reveal the limitations of the quasiparticle model and support a polaronic transport picture.
Moreover, we apply our workflow to the study of temperature-dependent bandgap renormalization in diamond, achieving results in excellent agreement with experimental data. These findings demonstrate the potential of the MLFF+SSCHA approach for studying quantum lattice dynamics and their impact on electronic properties.

Defense committee:
Samuel Poncé, UCLouvain, BE (reviewer)
Errea Lope Ion, Centro de Fisica de Materiales, ES (reviewer)
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