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ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Ab Initio Electron-Phonon Calculations: Theory, Computation, and Application to Carrier Dynamics

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Abstract: The interaction between charge carriers and lattice vibrations in solids, also known as electron-phonon (e-ph) interaction, controls a range of physical processes including charge transport, excited carrier dynamics, ultrafast spectroscopy and spin decoherence. Conventional e-ph calculations rely on empirical treatments that lack predictive power and quantitative accuracy. Ab initio calculations of the e-ph interaction using density functional theory and related methods are a recent focus in computational solid state physics; these novel e-ph calculations forego empirical parameters and can accurately predict materials properties controlled by e-ph processes.

This talk will introduce the theory of the e-ph interaction, together with its first-principles numerical implementation. Our recently developed algorithms to compute and interpolate the e-ph scattering rates will be presented. We will demonstrate application of e-ph calculations to charge transport and ultrafast excited carrier dynamics in metals, elemental and III-V polar semiconductors, and insulators. Presented results range from computing the resistivity and carrier mobility of a material with high accuracy to computing the dynamics and detailed scattering mechanisms of excited carriers. Code development efforts, open problems and future directions will be outlined.

Map: http://plan.epfl.ch/?room=med01418