Electron-phonon coupling from first-principles

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Abstract: For this seminar, I will highlight the importance of electron-phonon interaction to describe many experimental phenomena including carrier mobility, phonon-assisted optical absorption, phonon-limited superconductivity, zero-point renormalization, temperature dependence of the bandgaps, electron mass enhancement and polaron liquids.

I will show how to derive and efficiently compute electron-phonon interaction from first principles focusing on two manifestations of the electron-phonon coupling: carrier mobility and temperature dependence of the bandgap.

I will present the Boltzmann transport equation within the general framework of the quantum theory of mobility [1]. I will discuss the accuracy limit of ab initio electron-phonon limited calculations of carrier mobilities and show that predictive calculations of electron and hole mobilities require an extremely fine sampling of inelastic scattering processes in momentum space [2]. Such fine sampling calculation is made possible at an affordable computational cost through the use of efficient Fourier-Wannier interpolation of the electron-phonon matrix elements as implemented in the EPW code [3]. Using that interpolation technique, I will present recent findings on the intrinsic electron and hole mobility of silicon [2], wurtzite GaN [4], and halide perovskites [5].

Finally, I will discuss the Allen-Heine-Cardona (AHC) theory for the renormalization of the electronic bandstructure with temperature [6]. In particular, I will show that the adiabatic AHC theory allows for an easy computation of the effect of electron-phonon

interactions but cannot be used in the case of polar materials and will show results for Diamond, Si, a-AlN, b-AlN and BN [7].

References:

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About the speaker:

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