MAR17-2016-002922

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Anharmonic phonons and second-order phase-transitions by the stochastic self-consistent harmonic approximation[1]

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Anharmonic effects can generally be treated within perturbation theory. Such an approach breaks down when the harmonic solution is dynamically unstable or when the anharmonic corrections of the phonon energies are larger than the harmonic frequencies themselves. This situation occurs near lattice-related second-order phase-transitions such as charge-density-wave (CDW) or ferroelectric instabilities or in H-containing materials, where the large zero-point motion of the protons results in a violation of the harmonic approximation. Interestingly, even in these cases, phonons can be observed, measured, and used to model transport properties. In order to treat such cases, we developed a stochastic implementation of the self-consistent harmonic approximation valid to treat anharmonicity in the nonperturbative regime and to obtain, from first-principles, the structural, thermodynamic and vibrational properties of strongly anharmonic systems [1]. I will present applications to the ferroelectric transitions in SnTe, to the CWD transitions in NbS_2 and $NbSe_2$ (in bulk and monolayer) and to the hydrogen-bond symmetrization transition in the superconducting hydrogen sulfide system [2], that exhibits the highest Tc reported for any superconductor so far. In all cases we are able to predict the transition temperature (pressure) and the evolution of phonons with temperature (pressure).

[1] I. Errea, M. Calandra, F. Mauri, Phys. Rev. Lett. 111, 177002 (2013) and Phys. Rev. B 89, 064302 (2014)
[2] I. Errea, M. Calandra, C. J. Pickard, J. R. Nelson, R. J. Needs, Y. Li, H. Liu, Y. Zhang, Y. Ma, F. Mauri, Nature 532, 81 (2016)

[1]This project has received funding from the European Unions Horizon 2020 research and innovation programme under grant agreement No. 696656 GrapheneCore1