MAR17-2016-000752

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

Electronic structure of solids, including vibrational effects : Temperature dependence and zero-point motion.

XAVIER GONZE, Universite catholique de Louvain

Modifications of electronic eigenenergies due to vibrational effects and electron-phonon coupling are sizable in many materials with light atoms. While often neglected, they have been recently computed from first principles using different formalisms, among which the perturbation-based Allen-Heine-Cardona (AHC) approach, considering both the adiabatic and the non-adiabatic harmonic approximation. Electron-phonon coupling can be obtained from density-functional perturbation theory (DFPT) as well as from many-body perturbation theory (MBPT), e.g. the GW approximation. I will provide a brief overview of the concepts and formalisms, and present recent progresses, including : the validation of AHC theory implementation in two different software applications, with an agreed DFPT zero-point motion correction of 0.4 eV for the direct bandgap of diamond [1] ; the MBPT result for the same material, 40% higher [2]; the breakdown of the adiabatic AHC theory for infrared-active materials, and fix of this problem in the non-adiabatic AHC theory [3,4], with results for diamond, Si, LiF, AlN, BN, and a dozen oxydes; the connection with the Frohlich Hamiltonian and polaron physics. [1] S. Ponc, G. Antonius, P. Boulanger, E. Cannuccia, A. Marini, M. Ct and X. Gonze, Computational Materials Science 83, 341 (2014). [2] G. Antonius, S. Ponc, P. Boulanger, M. Ct and X. Gonze, Phys. Rev. Lett. 112, 215501 (2014). [3] S. Ponc, Y. Gillet, J. Laflamme Janssen, A. Marini, M. Verstraete and X. Gonze, J. Chem. Phys. 143, 102813 (2015). [4] G. Antonius, S. Ponc, E. Lantagne-Hurtubise, G. Auclair, X. Gonze and M. Ct, Phys. Rev. B 92, 085137 (2015).