Xavier Gonze[1], R. Caracas[1] and D. Klug[2]

[1]Université Catholique de Louvain
[2]Steacie Institute for Molecular Sciences, Ottawa

Linear-Response Identification of Phase Instabilities

The systematic idenfication of possible instabilities of a material can be done on the basis of the phonon band structure. Within density-functional theory, this band structure can be computed easily thanks to linear-response (density-functional perturbation theory). I will review the basis of this technique, and its implementation in the ABINIT software. Then I will present applications to high-pressure phase transitions (SiO_2, lithium), and to incommensurate phases (especially the Pb_2MgTeO_6 perovskite).