DFPT approach to the temperature dependence of electronic band energies[1] PAUL BOULANGER, MICHEL COTE, University of Montreal, XAVIER GONZE, Universite Catholique de Louvain — The energy bands of semiconductors exhibit significant shifts and broadening with temperature at constant volume. This is an effect of the direct renormalization of band energies due to electron-phonon interactions. In search of an efficient linear response DFT approach to this effect, beyond semi-empirical approximation or frozen- phonon DFT, we have implemented formulas derived by Allen and Heine [J. Phys. C **9**, 2305 (1976)] inside the ABINIT package. We have found that such formulas need a great number of bands, O(1000), to properly converge the thermal corrections of deep potential well atoms, i.e. elements of the first row. This leads to heavy computational costs even for simple systems like diamond. The DFPT formalism can be used to circumvent entirely the need for conduction bands by computing the first-order wave-functions using the self-consistent Sternheimer equation. We will compare the results of both formalism demonstrating that the DFPT approach reproduces the correct converged results of the formulas of Allen and Heine.

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