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Non-linear response of infinite periodic solids to homogenous electric fields and collective atomic displacements

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The non-linear response of infinite periodic solids to homogenous electric fields and cooperative atomic displacements will be discussed in the framework of density functional perturbation theory. The approach is based on the 2n + 1 theorem applied to an electric field dependent energy functional. We will focus on the non-linear optical susceptibilities, Raman scattering efficiencies and electrooptic coefficients. Different formulations of third-order energy derivatives will be examined and their convergence with respect to the k-point sampling will be discussed. The method will be applied to conventional semiconductors and to ferroelectric oxides. In the latter case, we will also describe how the first- principles results can be combined to an effective Hamiltonian approach in order to provide access to the temperature dependence of the optical properties. This work was done in collabration with M. Veithen and X. Gonze and was supported by the VolkwagenStiftung, FNRS-Belgium and the FAME-NoE.