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Phononic and nonlocality contributions to Second Harmonic Generation in NiO. WOLFGANG HUEBNER, GEORGIOS LEFKIDIS, Kaiserslautern University of Technology — The experimentally observed second harmonic signal in centrosymmetric NiO can be explained with symmetry lowering mechanisms: (i) signal from the surface, (ii) spin-orbit coupling, (iii) nonlocalities, and (iv) lattice distortions [1]. First the intragap energy levels of both the (001) surface and the bulk of NiO are obtained with highly correlated quantum chemistry methods: single excitation configuration-interaction, and multiconfigurational complete active space, optimizing each d-level separately. Then the second-order susceptibility tensor is calculated beyond the electric-dipole approximation. The effects of spin-orbit coupling are studied, and a detailed analysis of the effects of the inclusion of nonlocalities from magnetic dipoles and electric quadrupoles is performed. Finally the effects of phonons in the bulk of NiO within the frozen phonon approximation are included, and the second order susceptibility tensor is computed both in a time resolved and time averaged manner [2].

[1] G. Lefkidis and W. Hübner, Phys. Rev. Lett. 95, 77401 (2005).

[2] G. Lefkidis and W. Hübner, Phys. Rev. B 74, 155106 (2006).

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