Université catholique de Louvain UCL SECTEUR DES SCIENCES ET TECHNOLOGIES

Institut de la Matière Condensée et des Nanosciences

Invitation à la soutenance publique de thèse

Pour l'obtention du grade de Docteur en Sciences de l'Ingénieur

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Master ingénieur civil physicien

Ab Initio Study of Raman and Optical Spectra of Crystalline Materials and their Temperature Dependence

The strong dependence of Raman intensities with respect to the laser frequency is investigated thanks to the development of a first-principles methodology that relies on finite differences of the calculated dielectric function. This methodology is applied to the computation of the first-order frequency-dependent Raman intensity of silicon, gallium arsenide and silicon carbide, with excitonic effects described by the Bethe-Salpeter equation. We found these to be crucial for the accurate description of the experimental enhancement for laser photon energies around the gap. We also present a study on transition-metal dichalcogenides that reveals an atypical exciton-phonon interaction for WS_2 and WSe_2. This approach is generalized to the more complex second-order Raman intensity, with phonon losses coming from the entire Brillouin zone.

Temperature effects are also important for optical properties. Indeed, vibrations of the atoms induce temperature-dependent modifications of the band structure that, in turn, influence optical properties. In this work, we present a methodology for first-principles calculations of temperature-dependent band structure and optical properties, that is validated with respect to frequency-dependent and temperature-dependent Raman intensities of silicon.

Finally, all the techniques presented in this work are combined to analyze the more difficult case of multiferroic $BiFeO_3$. Recent experiments have shown strong laser-frequency dependence effects in Raman intensities but a small temperature dependence on first-order Raman. However, second-order Raman intensities show strong temperature dependence. Frequency-dependent Raman intensities and temperature-dependent band structures are computed and discussed.

Jeudi 5 janvier 2017 à 15h00

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Membres du jury :

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Prof. Bernard Piraux (UCL), président
Prof. Gian-Marco Rignanese (UCL), secrétaire
Prof. Philippe Ghosez (ULg)
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