Secteur des Sciences et Technologies

Invitation à la soutenance publique de thèse de

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Laurea Magistrali in Fisica

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« First-principles high-throughput study of linear and nonlinear optical materials »

qui se déroulera
le vendredi 30 août 2019 à 14h
Université du Luxembourg
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Batiment des sciences

Jury members :

Prof. Gian-Marco Rignanese (UCLouvain), supervisor
Prof. Ludger Wirtz (University of Luxembourg, Luxembourg), supervisor
Prof. Alexandre Tkatchenko (University of Luxembourg, Luxembourg), chairperson
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Nonlinear optical (NLO) processes, such as second harmonic generation (SHG), shift current, and others, play an important role in modern optics, especially in laser-related science and technology. They are at the core of a wide variety of applications ranging from optoelectronics to medicine. Among the various NLO materials, semiconductors are particularly important for second-order NLO properties. In particular, only crystals which are noncentrosymmetric can display a non-zero second-order NLO susceptibility. However, given the large number of requirements that a material needs to meet in order to be a good nonlinear optical material, the choice of compounds is drastically limited. Indeed, despite recent progress, a systematic approach to design NLO materials is still lacking. In this work, we conduct a first-principles high-throughput study on a large set of semiconductors for which we computed the linear and nonlinear susceptibility using Density Functional Perturbation Theory. We propose two main approaches for the analysis of the linear and nonlinear optical coefficients: (i) the analysis of the data trend through data mining techniques for the sake of deriving descriptive models, (ii) the screening of the materials collected in our databases to individuate interesting optical materials candidates. For the linear optical properties, our calculations confirm the general trend that the refractive index is roughly inversely proportional to the band gap. In order to explain the large spread in the data distribution, we have found that two descriptors successfully describe materials with relatively high refraction index: (i) a narrow distribution in energy of the optical transitions which brings the average optical gap close to the direct band gap (ii) a large number of transitions around the band edge and/or high dipole matrix elements. For non-centrosymmetric crystals, we perform the calculation of the efficiency of SHG. We observe some materials with particularly high SHG, much stronger than the general relation with the linear refraction index through Miller's rule predicts. We relate the value of Miller's coefficient to geometric factors, i.e., how strongly the crystal deviates from a centrosymmetric one. We also identified interesting materials that show high optical responses for which it would be worth performing further analysis.