Étude ab-initio dans le cadre de la DFT des propriétés structurales et physiques de supraconducteur à haute température critique (SHTc) de type pnictides de fer (FeSe)

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Abstract: In this work, we presented a study on the structural, elastic, electronic, magnetic and optical properties of iron selenide. The calculations were performed by the Pseudo-Potential method which is based on density functional formalism (DFT), using local density (LDA) and generalized gradient (GGA) approximations. The doped (GdFeSe and CeFeSe) and undoped (FeSe) structural properties such as the mesh parameters (a, b and c) and the compressibility modulus, are calculated as a function of pressure and the results found are in agreement with those advanced by the experimental and other calculations. In the study of the electronic properties of FeSe, the energy gap value calculated with the GGA approach are in agreement with those of other calculations. As far as the elastic properties are concerned, we calculated the elastic constants with the GGA approach and the found values of the latter are very close to those of the experiment. We also calculated the magnetic moment and confirmed that FeSe is a non-magnetic material. For the optical properties, we calculated the different optical properties such as the function of the reflectivity, the refractive index and the absorption coefficient.

Keywords : Superconductivity, pnictures, FeSe, DFT, pseudo potential, Castep