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A Comparative Study of the Effect of Strain on the Electronic and Optical Properties of Filled and Unfilled Ba_8Si_{46} Type I-clathrate

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A first principles calculations study is carried out to theoretically investigate the effect of compressive and tensile strains on the structural, electronic and optical properties of type-I guest-free Si_{46} and barium-filled Ba_8Si_{46} clathrates. The electronic band structure of the unfilled Si_{46} clathrate revealed a semiconducting behaviour with a quasi-direct band gap of 1.36 eV. Under hydrostatic pressure, the bandgap magnitude of the guest-free Si_{46} behaves monotonously. For the Ba doped Si_{46} clathrate (Ba_8Si_{46}) structure, the strain has no significant effect on the electronic band structure, while its impact on the optical properties is appreciable. The optical properties, such as the dielectric function and the absorption were computed for different strain variations, which are clearly enhanced for both the unfilled Si_{46} and Ba-filled Ba_8Si_{46} clathrates when the pressure is 1 GPa in the direction of a compressive state.

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1. Introduction

Group-IV inorganic clathrates are cage-like materials where a number of host atoms form a network arranged in cage shape to possibly enclose a guest atom. Indeed, this class of material is very promising given the large possibilities to tune the intrinsic properties by substituting both host and guest atoms in order to design new materials having desired functions for specific applications. Depending on the atomic arrangements eight types of clathrates are well established [1]. The type-I structure is the most investigated among the different known types, on the other hand, it has an excellent thermoelectric [1], semiconducting, and superconducting properties [2]. Guest free type-I Si_{46} silicon clathrate is a hypothetical structure, which has been theoretically studied and expected to exhibit interesting thermoelectric and electronic properties as a promising semiconductor material with a band-gap greater than that of silicon in the diamond structure [3]. However, the actual synthesis of type-I Si_{46} clathrate remains a challenging task and yet not resolved. In contrast with type-I Si_{46} silicon clathrate, the filled Ba_8Si_{46} [4] and partially vacant Ba_xSi_{46} [5] have been synthesized by different methods, mostly by using techniques based on high pressure and high temperature. The synthesized Ba_8Si_{46} material revealed several technological properties, especially it is known as the first clathrate to demonstrate low temperature superconductivity, in addition, by partial substitution of barium with aluminium, Ba_8Si_{46} have showed a good semiconducting behaviour [5]. One drawback of this material is related to its low mechanical properties under hydrostatic pressure.

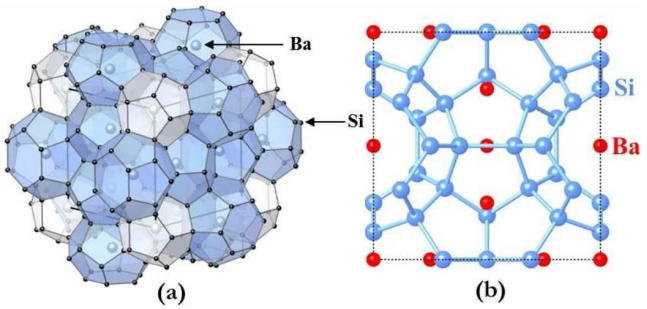

Fig. 1. Atomic configuration of Ba_8Si_{46} structure formed by polyhedrons network in (a) and the unit given in (b). Ba and Si atoms are shown respectively in red and in blue color.

In this work we have systematically investigated the effect of hydrostatic pressure on the electronic and optical properties of Ba_8Si_{46} and Si_{46} clathrates in type-I configurations by using first principles calculations in the frame of density functional theory (DFT). The development of the computational techniques for applying DFT to real materials has made it possible to predict quantitatively the atomic and electronic structure and properties of different materials [6–10]. In particular, the pseudopotential method based on the local DFT [7–11] has been very successfully used for studying various properties of the crystals [8], surfaces, and interfaces of metals, ceramics, and semiconductors [12]. The first part deals with