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Vacancy defect formation energies in Ba8@Ge46 clathrates KATSUHITO SAKAI, KAZUO TSUMURAYA, Meiji University — The clathrates I Ba8@Ge46 have been found experimentally to have vacancy defects in the framework and to form Ba8Ge43. This has been explained by the Zintl-Klemn empirical concept: the inclusion of the barium atoms leads to increase the valence electrons in the framework of the clathrates and the introduction of vacancy defects relaxes the hypervalence of the electrons. We clarify the process of the defect formation by analyzing the electric structure with the first-principle method. We calculate formation energy of a single vacancy in the clathrates in which we use Ceperley-Alder with LDA exchange correlation functional for the pseudopotential of barium atom.[J. Junquera et al. Phys.Rev.B 67,155327(2003)] The energies are 0.09eV for 6c, 0.39eV for 24k, and 0.74eV for 16i sites in the clathrate Ba8@Ge45, although 1.15eV for 6c, 1.31eV for 24k, and 1.70eV for 16i sites in the clathrate Ba8@Si45. The small energy of the 6c site is due to the small binding energy of Ge clathrate. We will present the reason why vacancy defects are introduced at the 6c sites.

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