

Abstract Submitted
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Peierls distortion of endohedral atoms in clathrate I HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji University, Japan — The guest atom displacements in type II clathrates have been reported on experimental and theoretical points of view. The displacements are reported to be 0.6 Å from the cage center of the Si₂₈ cage to the hexagonal in the hydrogen terminated double caged Si₂₈ cluster [1]. The distortion can be expected to occur in the type I clathrate which forms with bamboo structures in the x, y, and z directions. The guest atoms show Peierls distortion when we calculate the equilibrium distances between the two Na atoms which locate at the neighboring Si₂₄ cages in the bamboo structure using periodic density functional calculation. The binding energy between the guest atoms is -0.10 eV/Na₂. We also confirm the tendency of the Peierls distortion from the force directions of guest atoms in the double unit cells that contain four Na atoms in one dimension; We will propose the cohesion mechanism of the clathrates that the clathrates are precipitated states of the connecting endohedral atoms in the 14 group atoms. So are the hydroclathrates in which the guest molecules bind each other with chains. [1] H. Takenaka and K. Tsumuraya, Mater. Trans. 47, 63 (2006).

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