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Guest displacements in silicon clathrate II HIROYUKI TAKENAKA, Meiji University, KAZUO TSUMURAYA, Meiji University — Silicon clathrates are one of the candidates of the high performance thermoelectric materials due to their rattling effect of atoms in the cages. The clathrate II consists of Si20 and Si28 cages and the clathrate I Si20 and Si24 cages. Thus the clathrate II may have lower thermal conductivity than clathrate I. We investigate the stable position of the guest Na atom in the Si28 cage and the effect of nearest coordinated Na atoms in Si20 or Si28 cages on the displacements of Na atom in Si28 cage using the ab inito planewave method with pseudopotentials.

Hiroyuki Takenaka
Meiji University

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