Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Stabilities of earlier row atoms in group 1 and 2 for encapsulation in silicon clathrates I TOSHIHIKO OGURA, KAZUO TSUMURAYA, Meiji University — Group 14 clathrates consisting of Si, Ge, or Sn atoms have been synthesized only when they contain some specific endohedral atoms. They are Na, K, Rb, or Cs atoms in group 1, Sr or Ba atoms in group 2, and Cl, Br, or I atoms in group 17.[K.A.Kovnir, et al. Russian Chem. Rev.73,923(2004).] No experiment has been reported on the encapsulation of the earlier row atoms than the atoms mentioned above. We predict the stability of the encapsulation of these atoms using ab initio methods. We evaluate the stability of the guest atom in double caged M2@Si42H36 cluster in the clathrate I, where M is group 1, 2, or 17 atom. The encapsulation of two lithium atoms into one cage and the other is vacant is more stable than the separate encapsulation of lithium atoms into each cage by 0.436eV. The Be2 is the same case and by 0.0859 eV. For sodium case, the separate encapsulation into each cage is more stable by 1.473eV. The strong dimer formation prevents the stabilization of the cage structure. We also evaluate the stabilities in the crystalline states.

Toshihiko Ogura
Meiji University

Date submitted: 03 Dec 2005 Electronic form version 1.4