Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic structures and displacements of endohedral sodium atoms in silicon clathrate II HIROYUKI TAKENAKA, KAZUO TSUMURAYA, Meiji University — Since group 14 clathrates encapsulate specific atoms in their cages, the atoms give rise to rattling motion in the cages leading to low thermal conductivity. The clathrate II consists of Si_{28} and Si_{20} cages and the Si_{28} cage is the largest among the cages in the clathrates. We investigate the displacements and the charge densities between the endohedral sodium atoms in the clathrate II using ab initio methods. First we present the displacements of the guest sodium atoms in double caged $Na_2@Si_{50}H_{44}$ cluster, which is a piece of clathrate II being hydrogenated in order to terminate the dangling bonds. Although in a single $Si_{28}H_{28}$ cage the endohedral sodium atom is the most the most stable at the center of the cage, the sodium atoms in each of the double cage cluster displace about 0.06 nm away from each center of the cages to shorten the distance of the sodium atoms. The displacements are attributed to the formation of covalent bond between the sodium atoms and the ionic bonding between the sodium atoms and the cage silicon atoms. Secondly we present the bonding charge densities between the sodium atoms in the clathrate II.

Hiroyuki Takenaka
Meiji University

Date submitted: 15 Jan 2006 Electronic form version 1.4