Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Binding Energies between Guest Atoms in Clathrate II
HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji University, JAPAN — The guest atom displacements in clathrates II have been reported on experimental and theoretical points of views. The recent papers on the displacements are given in the reference [1]. The displacements are found to be about 0.6 Å from the center of the Si_{28} cage to the hexagonal ring between the Si_{28} cages. The binding energies between the guest atoms however have been unknown so far. In the present work we calculate the energies between Na atoms in clathrates II $Na_2@Si_{136}$ and $Na_{24}@Si_{136}$ with a density functional analysis. We will discuss the cohesion mechanism of the clathrates based on the binding nature between the cations in Zintl phase. [1] H. Takenaka and K. Tsumuraya, Mater. Trans., 47, 63 (2006).

Hidekazu Tomono
Meiji University, JAPAN

Date submitted: 20 Nov 2006 Electronic form version 1.4