

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Roll of dimer formation in crystallization of clathrate I: from clusters to crystal KAZUO TSUMURAYA, TAKEHARU AOI, TOSHIHIKO OGURA, Meiji University — Silicon clathrates are metastable and have been synthesized only when alkaline or alkaline earth metal atoms coexist as electron donors or VIa or VIIa atoms coexist as electron acceptors. These guest atoms locate in the cages of the crystals. Now, however, the roll of the guest atoms is unclear in the crystallization processes. We investigate it through investigating the coagulation processes between the cage clusters. We use ab initio electronic structure analysis in real space and the one in momentum space. The formation of dimers between the guest atoms is found to be essential in the synthesis.

Kazuo Tsumuraya
Meiji University

Date submitted: 06 Dec 2004

Electronic form version 1.4