Contribution ID: **5** Type: **not specified**

A novel method to predict densities of amorphous materials from first-principles calculations

Tuesday, 20 June 2017 15:30 (15 minutes)

First-principles calculations had not ever been performed to predict the densities of amorphous materials. This was due to the fact that because of the disordered nature of amorphous materials, their atomic configurations are completely different from one sample to another, and thus there is no one-to-one correspondence between the densities and the total energies. In our study, to remedy this problem, we have devised a novel method which employs the density functional theory (DFT) and the Car-Parrinello molecular dynamics method based on the DFT. We have applied it to amorphous silicon and found that the determined density and its bulk modulus are in good agreement with experiment. The results suggest the validity of the proposed method.

Primary author: Mr FURUKAWA, Yoritaka (The Univesity of Tokyo)

Co-author: Dr MATSUSHITA, Yu-ichiro (The University of Tokyo)

Presenter: Mr FURUKAWA, Yoritaka (The Univesity of Tokyo)