

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Novel Be-intercalated Hexagonal Boron Layers Structure of BeB₂

KAI-MING HO, MANH CUONG NGUYEN, XIN ZHAO, CAI-ZHUANG WANG, Iowa State University — Using genetic algorithm method and first-principle calculations, we performed searches for low-energy crystal structures of BeB₂. We found a new family of structures, where the B atoms form hexagonal layers intercalated by Be atoms. The lowest-energy structure has formation energy of -99.47 meV/atom with 4 formula units in the unit cell, which is much more stable than the models proposed before. The formation energies of structures in the new structure family can be well described by a Ising-like model with “anti-ferromagnetic” coupling between the displacements of Be atoms from the mid-plane between two B layers. We also performed phonon calculation as well as electronic band structure calculation to verify the stability and investigate the electronic properties of the newly found ground-state structure.

Xin Zhao
Iowa State University

Date submitted: 15 Nov 2013

Electronic form version 1.4