第71回フロンティア材料研究所講演会
71st MSL Lecture

Date/Time: 11:00 - 12:00, Monday, August 6th, 2018

Venue: 1F Meeting Room, Building R3

Speaker: Dr. Ha-Jun Sung

Department of Physics,
Korea Advanced Institute of Science and Technology (KAIST)

Computational materials search for novel metallic C and Si allotropes using an inverse design method

With the recent advance of computational power, discovery and design of new materials are being revolutionized by computational materials science. Recently, we have developed a protocol for a crystal structure search, in which the conformational space annealing algorithm for global optimization is combined with first-principles density functional calculations, called AMADEUS [1]. The AMADEUS has been successfully used to predict new materials, such as silicon and carbon allotropes with optimal direct band gaps for photovoltaic applications, possible intermediate phase of boron on the transition pathway from *α*-B to *γ*-B, a new phosphorus allotrope called green phosphorus with high carrier mobility, and a two-dimensional triangular Kagome lattice of boron that exhibits the exotic electronic properties.

In this presentation, we will show the successful application of AMADEUS to predict a novel metallic allotropes of carbon [2] and silicon [3]. The new carbon allotrope, termed *m*-C_8, consists of five-membered rings with sp^3 bonding interconnected by sp^2-bonded graphitic carbon networks. Analyzing the electronic band structure, we identify that *m*-C_8 belongs to the class of topological nodal line semimetals. The new Si allotrope, termed *P6*/*m*-Si_6, contains open channels embedded in a simple hexagonal lattice. The new Si_6 phase can be obtained by removing Na atoms from a chemical precursor $NaSi_6$ in the *P6*/*m* space group that is discovered using AMADEUS at high pressure. We find that both the *P6*/*m*-Si_6 and *P*6/*m*-Si_6 clathrates are stable and superconducting with the critical temperature of about 12 and 13 K at zero pressure, respectively.

References
[1] I.-H. Lee, Y. J. Oh, S. Kim, J. Lee, and K. J. Chang, *Comp*. *Phys*. *Commun*. **203**, 110 (2016).
[2] H.-J. Sung, S. Kim, I.-H. Lee, and K. J. Chang, *NPG Asia Mater.* **9**, e361 (2017).
[3] H.-J. Sung, W. H. Han, I.-H. Lee, and K. J. Chang, *Phys. Rev. Lett.* **120**, 157001 (2018).

Sung博士は、KAISTのKee Joo Chang教授のグループにおいて、結晶構造探索アルゴリズムによる新規結晶構造の理論予測を行っています。本講演では、金属的な電子構造を示すCやSiの多形の予測を中心にお話しいただきます。ぜひご参加ください。

Contact: Fumiyasu Oba (ext. 5511)