New Carbon Allotropes: Materials Design and Photocatalysis Application

Hiroshi Mizuseki [1]
[1] *Korea Institute of Science and Technology (KIST), Hwarangno 14-gil 5, Seongbuk-gu, Seoul 02792, Republic of Korea*

The search for new carbon allotropes by using theoretical approaches is an important subject in the field of computational materials science. Many allotropes of carbon across dimensions possess a wide range of properties and applications, due to its ability to form sp, sp^2, sp^3 and sp^2+sp^3 - hybridized chemical bonds. With advances of synthetic tools and simulation approach, a variety of novel carbon allotropes were obtained or predicted. In this presentation, we will discuss our simulation results of two-dimensional carbon allotropes for photocatalysis application [1] and discuss new methodology for prediction of new carbon structures based on a combination of evolutionary approach and atomistic simulation based on Tersoff potential and first-principles calculation.

We are grateful for the financial support from the Korea Institute of Science and Technology (Grant No. 2E26940). This study was also partly supported by the computational resources of the HPCI system (Project ID: hp170190) and the inter-university cooperative research program of Institute for Materials Research, Tohoku University (Proposal No. 17S0007), Japan.

References:

[1] Babu Ram and Hiroshi Mizuseki, in preparation

Email: mizuseki@kist.re.kr