The 21st Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-21)

October 29 — 31, 2018
Fusion Hall, KI Building
KAIST
Daejeon, Korea

KAIST

APCTP
Asia Pacific Center for Theoretical Physics

Poster-116

Vibrational effects on the surface energy of III-V compound semiconductors using ab-initio thermodynamics

In Won Yeu[1,2], Gyuseung Han[1,2], Cheol Seong Hwang[2], and Jung-Hae Choi[1,*]

[1]*Center for Electronic Materials, Korea Institute of Science and Technology, Seoul 02792, Korea*
[2]*Department of Materials Science and Engineering, and Inter-university Semiconductor Research Center, Seoul National University, Seoul 08826, Korea*

[*] E-mail: choijh@kist.re.kr

The surface energy is important in understanding the surface structure and crystal shape which are crucial to design materials for various applications. The conventional density functional theory (DFT) provided a method to obtain the surface energy, γ, as a function of chemical potential, μ. One of the main difficulties of using $\gamma(\mu)$ is that it cannot be directly compared with the experimental results because (i) $\gamma(\mu)$ is the electronic energy difference of the ground state; (ii) it is almost impossible to control μ through the experimental variables of temperature (T) and pressure (P); and (iii) the surface vibrational and configurational entropy effects which are calculated as a function of T cannot be consistently combined with $\gamma(\mu)$.

We reccently estabilished a thorough method to calculate the surface energy as a function of T and P by combining DFT and thermodynamics [1]. In addtion, the surface energy including the effects of surface vibration was obtained for the typical III-V compounds, such as GaAs and InAs by considereing various reconstructions with different stoichiometry and bonding geometry. As a result, we confirmed that some reconstructions which are unstable in terms of electronic surface energy become energetically stable at high T due to the surface vibrational effects. The calculation results were compared with the previous experimental works and showed good agreements. Such a correspondence of the calculations and experiments for a given T and P has not been available in the previous DFT calculations.

[1] In Won Yeu *et al.* Sci. Rep. **7**, 10691 (2017).