**Phase Diagram of Ga(As,Sb) and (In,Ga)As   
by Cluster Expansion and DFT Calculations**

Gyuseung Han,1,2 In Won Yeo,1,2 Seung Cheol Lee3, Cheol Seong Hwang1 and Jung-Hae Choi2,\*

*1Center for Electronic Materials, Korea Institute of Science and Technology, Seoul 02792, Korea*

*2Department of Materials Science and Engineering, and Inter-university Semiconductor Research Center, Seoul National University, Seoul 08826, Korea*

*3Indo-Korea Science and Technology Center, Bengaluru 560065, India*

\* E-mail: [choijh@kist.re.kr](mailto:choijh@kist.re.kr)

A solid solution is a chemical mixture of several components and forms a single phase in a certain range of composition. For a given composition of a solid solution, tremendous number of atomic cofigurations are possible and properties of a solid solution depend on the configuration [1][2]. Therefore, it is practically impossible to calculate the all possible configurations by DFT calculations. On the other hand, materials properties come from the interaction between atoms, and the properties of materials can be interpreted as the sum of the contribution of interactions of some atomic groups, which are called clusters. Cluster expansion method predicts the properties of any atomic configuration by calculating the contribution of each interaction on properties [3]. Predicted properties of each configuration are combined into properties of materials by the grand canonical ensemble.

In this study, the phase diagrams of Ga(As,Sb) and (In,Ga)As are calculated by the combined methods using ab-initio calculation, cluster expansion, canonical ensemble and grand canonical ensemble. Although Ga(As,Sb) and (In,Ga)As systems have been studied as one of the promising next-generation semiconductor channel materials, experimental studies on the phase diagram of (In,Ga)As have been rare [4] and the those on Ga(As,Sb) show ambiguous results [5][6]. we provide the phase diagrams of Ga(As,Sb) and (In,Ga)As phase and compare them with the previous experimental and theoretical results.

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