Structural stability and electronic states of AA and AB stacked II-V compounds

L. G. Arellano[1,2] and J. Nakamura[1]

[1] *Department of Engineering Science, The University of Electro-Communications (UEC Tokyo), 1-5-1 Chofugaoka, Chofu, Tokyo 182-8585, Japan*
[2] *1Instituto Politécnico Nacional, ESIME Culhuacán, Av. Santa Ana 1000, Ciudad de México, México*

lucyarellano.ipn@gmail.com

Various 2D semiconductor thin films have been available. Due to the surface and the quantum confinement effects, these 2D materials exhibit different electronic properties [1-3]. Recent studies have demonstrated that double-bilayer compounds (DB-C) from the II-V group, CdAs-164 (AB stack) and CdAs-187 (AA stack), are stable using first-principles calculations (FPC) [4]. On the other hand, we have recently revealed that various II-V DB compounds are stable in a different stacking fashion, AB' [5]. In addition, it has been concluded that the AB-stacked CdAs and CdP exhibit topological properties showing metallic behavior [5]. The purpose of this study is to evaluate the structural stability and electronic structure of the AA and AB stacking (see Fig. 1.) of DBC consisting of group II (Be, Zn, Cd) and group V (P, As, Sb) systematically using (FPC) based on the density functional theory.

The AB stack has greater stability when compared with the AA, except for BeSb, although there is little difference in energy between them. Due to greater Coulomb repulsion between atoms within the same group, the distance between layers in AA stack is greater than that in AB. Recently, we have revealed that the structural stability of the II-V DB-C depends strongly on the difference in atomic radius between the II and V group atoms; Atoms with larger radii are always located at the top surface. Such a size effect also affects the surface structure and the structural stability of AA and AB in the same way as AB'. However, in the AA and AB stacks, group V atoms form strong covalent bonds between BLs. As a result, group II atoms are always located on the top surface. Cd and Zn structures with a larger atomic radius tend to be on the surface and, therefore, have metallic properties. In contrast, Be, a smaller atom, tends to form flat structures and semiconductors. Consequently, it can be concluded that the covalent bonding between layers determines the stability of the II-V DB-C.

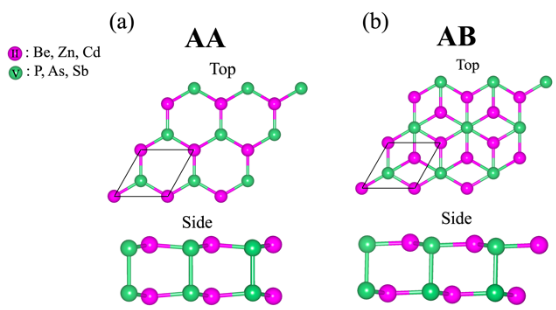

Fig. 1. Top and side views of initial structures of DB-stacked II-V compounds. (a) AA-stacking and (b) AB-stacking.

[1] Kailiang Zhang, *et al*., J. Mat. Chem., 5, 11992-12022 (2017).
[2] Hannu-Pekka Komsa, *et al*., J. Phys. Chem. Lett., 3, 3652-3656 (2012).
[3] Shoichi Takasuna, *et al*., Phys. Rev. B., 96, 161303 (2017).
[4] Yan, Quihui, *et al*., J. Phys. Condens. Matter, 33, 36-365701 (2021).
[5] Arellano, L. G., *et al.,* Phys. Rev. Mater., 7, 1, 014006 (2023).