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HSE hybrid functional calculation of absolute deformation potential in $MgGeN_2$

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The ternary wide band gap semiconductor, $MgGeN_2$ is one of the group II-IV-N_2 compounds which have recently become potential alternatives for the group III-N materials. This is as the II-IV-N_2 has two different cations, so its electronic properties can be modified/tuned by varying the concentration of the group II or IV elements. The crystal structure of II-IV-N_2 can be considered as the super lattice of wurtzite structure, so the heterojunction between II-IV-N_2 and other wurtzite semiconductors (for example GaN and ZnO) is possible to synthesize. Therefore, it is customary to preliminarily acquire the potential-change associated lattice deformation (arisen from the lattice mismatch), via the investigation of absolute deformation potential (ADP). The ADP is the energy level shifting due to the distorted lattice. This potential is very important to extract the electronic properties in heterojunction semiconductors. In this work, we calculated the ADP of the valence band maximum (VBM), conduction band maximum (CBM), and energy gap of $MgGeN_2$. The $MgGeN_2$ was considered as a prototypical investigating material due to its less lattice mismatch comparing to GaN and ZnO. In extracting the ADP, the derivative of the energy with respect the logarithmic volume was carried out, where in this work the volume deformation was allowed to range between -2% to 2% of the experimental bulk $MgGeN_2$. Then, VBM, CBM and band gap were obtained using the Heyd-Scuseria-Ernzerhof hybrid functional (HSE) approach. The average electrostatic potential in each semiconductor was considered as a reference energy level instead of the core level, which is suitable for Norm-Conversing Pseudopotential approach used in this work. Then, the ADP and related results of the $MgGeN_2$ were also compared with the well-known GaN and ZnO. We found that the trend of energy shift due to strain in $MgGeN_2$ is larger than that of GaN and ZnO. These results of ADP therefore reveal energy shift characteristic associated to volume deformation, which could be useful for designing semiconductor applications based on the group II-IV-N_2 compounds.

Primary author: KAEWMEECHAI, Chaiyawat

Co-authors: PUNYA JAROENJITTICHAI, Atchara; LAOSIRITAWORN, Yongyut

Presenter: KAEWMEECHAI, Chaiyawat

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