Structural stability of 2D II-V compounds

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After the discovery of graphene, research to develop new 2D materials has been vigorously pursued. Currently, other 2D materials like hexagonal Boron Nitride, transition metal dichalcogenides such as MoSe and III-VI compound semiconductor thin films can be available. These 2D materials have different electronic properties such as bandgap[1-3], at the same time have different physical properties from those that exist in bulk, due to their surface and quantum confinement effects.

In a recent study, it was reported that three-dimensional ZnSb with a layered structure can be fabricated by electrochemical treatment of ZnSb, an II-V compound semiconductor, and also theoretically suggested that ZnSb ultrathin films, which are the building blocks of the layered ZnSb structure, can exist stably [4].

This study will evaluate the structural stability of ultra-thin films of Group II-V compounds, whose existence has not been confirmed not only experimentally but also theoretically. The possibility of their existence will be explored through first-principles calculations based on the density functional theory. Analyzing the electronic structure and structural stability of group II (Be, Zn, Cd) and group V (P, As, Sb) compound ultrathin films. Its structural stability is also checked by phonon calculations.

The results show that the formation energy was found to be positive for BeP, BeAs, ZnP, and ZnAs, *i.e.*, the reaction was exothermic and thermodynamically stable. Also through phonon calculations, no imaginary frequencies were found in all the aforementioned compounds and ZnSb, which confirms their structural stability and in turn its possible existence.

References:

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