Heteroepitaxial growth of III-V on Si: a DFT perspective

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Understanding the physical properties of heterogeneous integration, such as the epitaxial growth of III-V on Si, is highly desirable for more advanced and futuristic optoelectronic and photoelectric applications of semiconductors [1, 2]. Using density functional theory, we first demonstrate how it is possible to investigate the absolute surface and interface energies with the variations of chemical potential for heterogeneous materials systems [3, 4]. Then, we show how to quantify the impact of Si surface passivation before III-V/Si hetero-epitaxy on the surface energy of the Si initial substrate, which plays an essential role in establishing its wetting characteristics on the specific case of GaP/Si [5]. In addition, we highlight that this inevitable passivation leads to a considerable reduction of the substrate surface energy, which in turn leads to a significant decrease in spreading parameters and evidence the heteroepitaxy in 3D Volmer-Weber type. Finally, we explore the possibilities to have a full *ab initio* description of Wulff-Kaishew equilibrium morphology prediction.

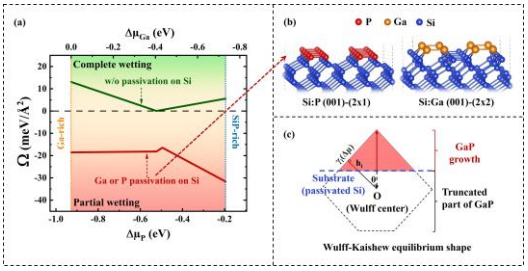

Fig.1. (a) Spreading parameter determined from DFT calculations on GaP/Si (b) Si surface passivation atomic structure, and (c) illustration of the Wulff-Kaishew equilibrium shape.

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