Black Phosphorene Like α-SiS with Robust Photovoltaics Properties

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The field of condensed matter physics has been experiencing a rapid development of the two-dimensional (2D) materials family. When going from initial materials discoveries to potential device applications, the success of each of the enigmatic 2D system depends critically on the development of efficient and scalable methods for epitaxial growth of large-area and high-quality crystalline samples on proper substrates. Yet to date, the spotlighted 2D systems, black phosphorene like α-SiS has not been grown despite extensive efforts on exploring epitaxial growth, largely due to the failure to identify fertile substrates that can promote its epitaxial growth. In this attempt, we deliver a solution to this standing challenge by proposing a straightforward yet conceptually intuitive approach for fabricating α-SiS via epitaxial growth. Our substrates of choice are the few layers black phosphorene (BlackP) substrate that possesses both structural and chemical affinities [1, 2]. Based on van der Waals (vdW) corrected first-principles approaches, that α-SiS is energetically and thermodynamically stable on BlackP (001) as the representative substrate, this aspect is highly desirable for initial growth and eventual mass production of α-SiS. Based on the HSE06 functional the α-SiS/BlackP vdW heterostructure manifests semiconducting properties with an indirect band gap 1.61 eV. The AIMD simulations up to 900 K for 5 ps to confirm the thermodynamic stability of α-SiS/BlackP vdW heterostructure [3]. We have characterized the kinetic stability of α-SiS/BlackP vdW heterostructure by calculating the phonon dispersion via DFPT methods [4]. Moreover, the α-SiS/BlackP vdW heterostructure possesses high optical absorption strength $\sim 10^5$ cm^{-1}, and can effectively harvest visible solar radiation. The wavelength-dependent optical absorption coefficient $\alpha(\omega)$ is calculated for the α-SiS/BlackP vdW heterostructure and the corresponding isolated α-SiS and BlackP monolayers using HSE06 method. It can be seen (Fig. 2(d)) that the α-SiS/BlackP vdW heterostructure optical absorption around 400 nm (favorable solar harvesting region) is more noticeable than that of the constituent BlackP and α-SiS monolayers. In addition, the α-SiS/BlackP vdW heterostructure exhibits widespread optical absorption spanning from infrared to visible light, and the optical absorption intensity can reach the order of 10^5 cm^{-1}. These findings demonstrate that integrating the α-SiS monolayer with the BlackP monolayer significantly boosts their efficiency in solar energy harvesting and photodetection. The α-SiS growth on such semiconducting substrates could become a novel platform for next-generation nano-energy technology.

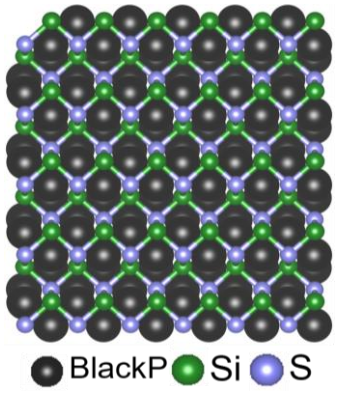

Figure 1. Epitaxial growth of α-SiS on few layers black phosphorene substrate.

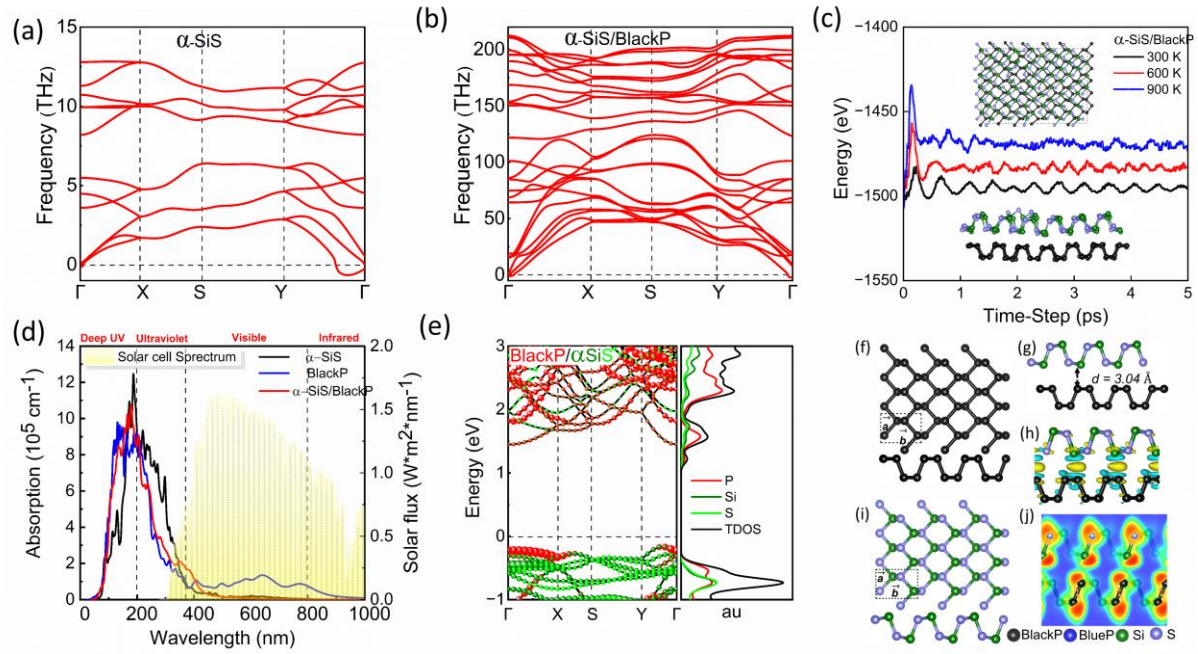

Figure 2. Phonon spectra of the (a) α-SiS monolayer, (b) α-SiS/BlackP vdW heterostructure calculated with DFPT. (c) Total energy evolution during the AIMD simulations up to 900 K and up to 5.0 ps, indicating that the α-SiS/BlackP vdW heterostructure is stable up to 900 K; (d) Optical absorption spectra of the α-SiS/BlackP vdW heterostructure; (e) Electronic band structure (left) and density of states (right) of α-SiS/BlackP vdW heterostructure. Top and side views of geometric structure of (f) BlackP, (i) α-SiS monolayer, where the dotted rectangle denotes the unit-cell of the freestanding monolayer. (g) Side view of α-SiS/BlackP vdW heterostructure; (h) charge density differences of α-SiS/BlackP vdW heterostructure. The isosurface value is set to 0.0005 eÅ^{-3}. The ELF contour plots of the (100) crystal plane of (j) α-SiS/BlackP vdW heterostructures.

Keywords：black phosphorene; α-SiS; isoelectronic; isostructural; first-principles calculations

References

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BIOGRAPHY

Nisar Muhammad was awarded his Bachelor's degree by the University of Peshawar. He obtained Master's degree from the University of Science and Technology of China and is now a PhD student under supervision of Professor Ding Zejun. His research is centered on the first-principle prediction and investigation of nanomaterials.

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