Raman response, piezoelectricity, and transport properties of the two-dimensional Janus HfSiX_3H (X = N/P/As) semiconductors: A first-principles study

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Exploring advanced materials with extraordinary properties is necessary for developing high-performance devices. In this work we construct two-dimensional Janus HfSiX_3H (X = N/P/As) monolayers and systematically examine their physical properties by utilizing first-principles calculations. Specifically, we focus on the stabilities, Raman spectra, electronic structures, piezoelectricity, and transport properties of the monolayers. As a result, the studied $HfSiN_3H$, $HfSiP_3H$, and $HfSiAs_3H$ monolayers are found as semiconductors with good structural, mechanical, dynamic, and thermodynamic stabilities. The piezoelectric coefficients (e_{11} and e_{31}) are calculated to examine the piezoelectricity of the HfSiX_3H monolayers. It is noted that besides the in-plane piezoelectricity, the three monolayers show additional out-of-plane piezoelectric effects because of their noncentrosymmetric structures. We also include fully anisotropic acoustic deformation potential, ionized impurity, piezoelectric, and polar electron–phonon scattering to calculate the total carrier mobilities of Janus HfSiX_3H. It is demonstrated that Janus HfSiX_3H monolayers exhibit low carrier mobilities at room temperature (<100 cm^2 V^{-1} s^{-1}). Scattering from polar optical phonons is found to dominate the total mobilities of both electrons and holes.

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I. INTRODUCTION

The exploration of two-dimensional (2D) layered nanomaterials has opened more opportunities for the utilization of advanced materials in innovative applications. In the past two decades, numerous 2D layered materials have been reported such as antinonene [1], transition-metal oxides [2], transition-metal monochalcogenides [3,4], MXenes [5], black phosphorous [6], or bismusthene [7]. 2D materials have been predicted to have superior physical and chemical properties compared to their bulk counterparts [8–10]. Particularly, recently 2D Janus materials with vertically asymmetric structures have been experimentally reported [11,12], making the 2D family more diverse. Owing to asymmetric structure, the 2D Janus materials exhibit various extraordinary features for potential applications in electronics [13], optoelectronics [14], thermoelectrics [4,15], catalysis [16], and sensors [17].

Recently, a series of MA_2Z_4 materials (M refers to transition-metal, A corresponds to Si or Ge, and Z is N/P/As) have been discovered with many attractive properties. For example, Cai *et al.* explored Janus MoAZ_3H monolayers (with A = Si/Ge and Z = N/P/As) by using first-principles calculations. They found the spin-valley coupling enhancement of the MoAZ_3H with different A and Z elements. The out-of-plane and in-plane piezoelectricity were also found in the studied monolayers. Thus both piezoelectric and valleytronic properties coexisted in the MoAZ_3H monolayers. Notably, these piezoelectric and valleytronic properties could be tailored by the presence of strain [18]. Deng theoretically studied the Raman spectra of $MoGe_2As_4$, $TiSi_2N_4$, and $MoSi_2N_4$ monolayers modulated by an electric field. The angle-dependent Raman intensity of the three monolayers was determined by using the density functional theory. It was seen that the symmetry of D_{3h} was reduced to C_{3v}, leading to more Raman-active mode peaks by applying an external electric field to the $MoSi_2N_4$. This enhancement on Raman spectra was about ten times [19]. Liu and co-workers proposed 2D Janus $WSiGeZ_4$ (Z = N/P/As) materials and investigated their photocatalytic and electronic properties by strain engineering. They found that the photocatalytic and electronic properties of the monolayers were sensitive when the Z element changed from N to As. In addition, the biaxial strain caused direct-indirect band gap and semiconductor-metal transitions and modulated the optical and photocatalytic properties of the $WSiGeZ_4$ materials [20]. A research group of Gou predicted Janus $MSiGeN_4$ (M = Zr and Hf) structures with good thermal and mechanical stabilities. The applied strains could induce phase transformation from a

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