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RESEARCH ARTICLE

Two dimensional $GeO_2/MoSi_2N_4$ van der Waals heterostructures with robust type-II band alignment

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Supporting Information

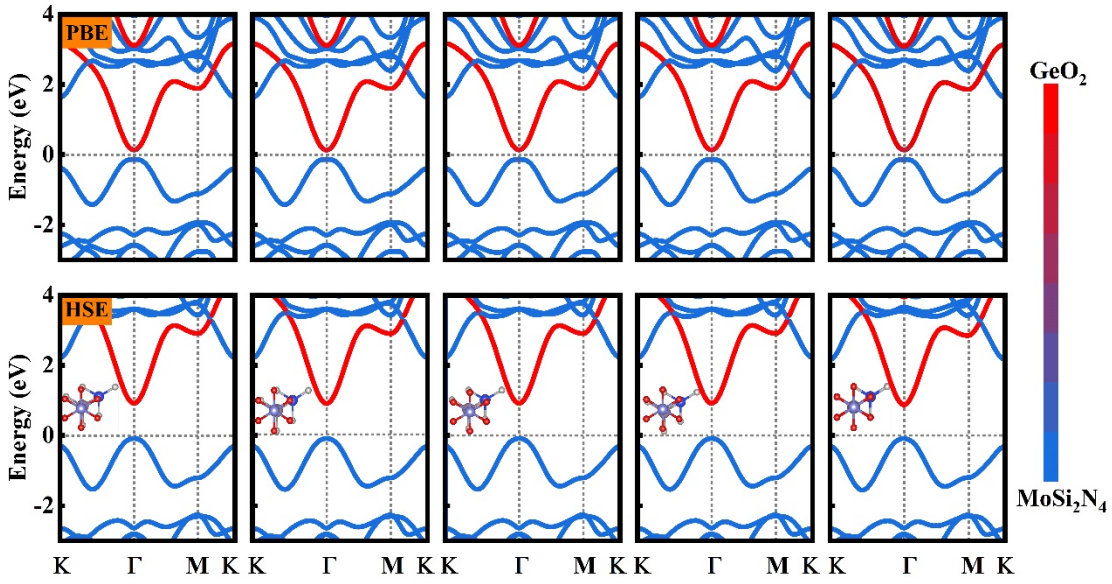

Fig. S1 The layer-dependent projected electronic band structures of metastable and most stable geometric structures of $GeO_2/MoSi_2N_4$ vdWHs using PBE (up) and HSE06 (bottom). The inset is a top view of the corresponding geometry structures. From left to right, the structures are defined as structure-I, II, III, IV, and V (the most stable).

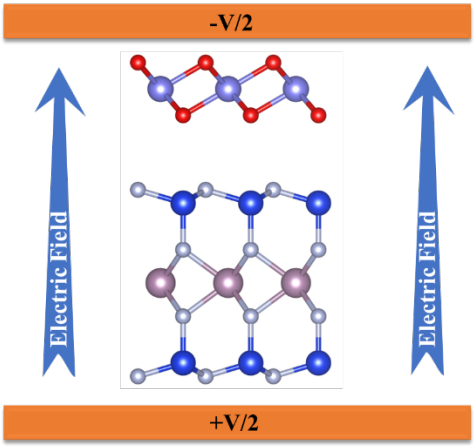

Fig. S2 Schematic model of the $GeO_2/MoSi_2N_4$ vdWHs in the case of external electric field.

Figure S1 shows the layer-dependent projected electronic band structures for the metastable and most stable $GeO_2/MoSi_2N_4$ vdWHs. For convenience, the metastable structures and most stable structures are defined as structure-I, II, III, IV, and V. These configurations are all eclipsed by stacking with the O over Si, O over N and Ge over Mo. However, among them, only structure-V is stacked with the atomic centers facing each other. The layer-dependent projected electronic band structures of the structure-I, II, III, IV, and V demonstrate a type-II band alignment with the CBM and VBM contributed by GeO_2 and $MoSi_2N_4$. The E_g of these five constructions calculated by PBE (HSE06) are 0.274 (0.999) eV, 0.271 (0.993) eV, 0.275 (0.997) eV, 0.276 (1.000) eV, 0.275 (0.946) eV, respectively. Furthermore, the CBM and VBM of these five configurations are located in the Γ point, forming a direct band gap. Thus, there is little difference in the total energy between the different stacking patterns of each heterostructure, and the band structures of five stacking patterns are very similar.

Table S1 The lattice constant (a), interlayer distance (d), total energy (E_{total}), band gap of PBE (E_g^{PBE}) and HSE06(E_g^{HSE06}), and locations of the CBM and VBM in the k space.

	a (Å)	d (Å)	E_{total} (eV)	E_g^{PBE} (eV)	E_g^{HSE06} (eV)	CBM/VBM
Structure-I	2.909	2.87	-82.815	0.274	0.999	Γ/Γ
Structure-II	2.909	2.87	-82.815	0.271	0.993	Γ/Γ
Structure-III	2.909	2.86	-82.815	0.275	0.997	Γ/Γ
Structure-IV	2.909	2.86	-82.815	0.276	1.000	Γ/Γ
Structure-V	2.909	2.78	-82.816	0.275	0.946	Γ/Γ