Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information (SI)

Band alignment and optical features in Janus-MoSeTe/X(OH)$_2$ (X = Ca, Mg) van der Waals heterostructures

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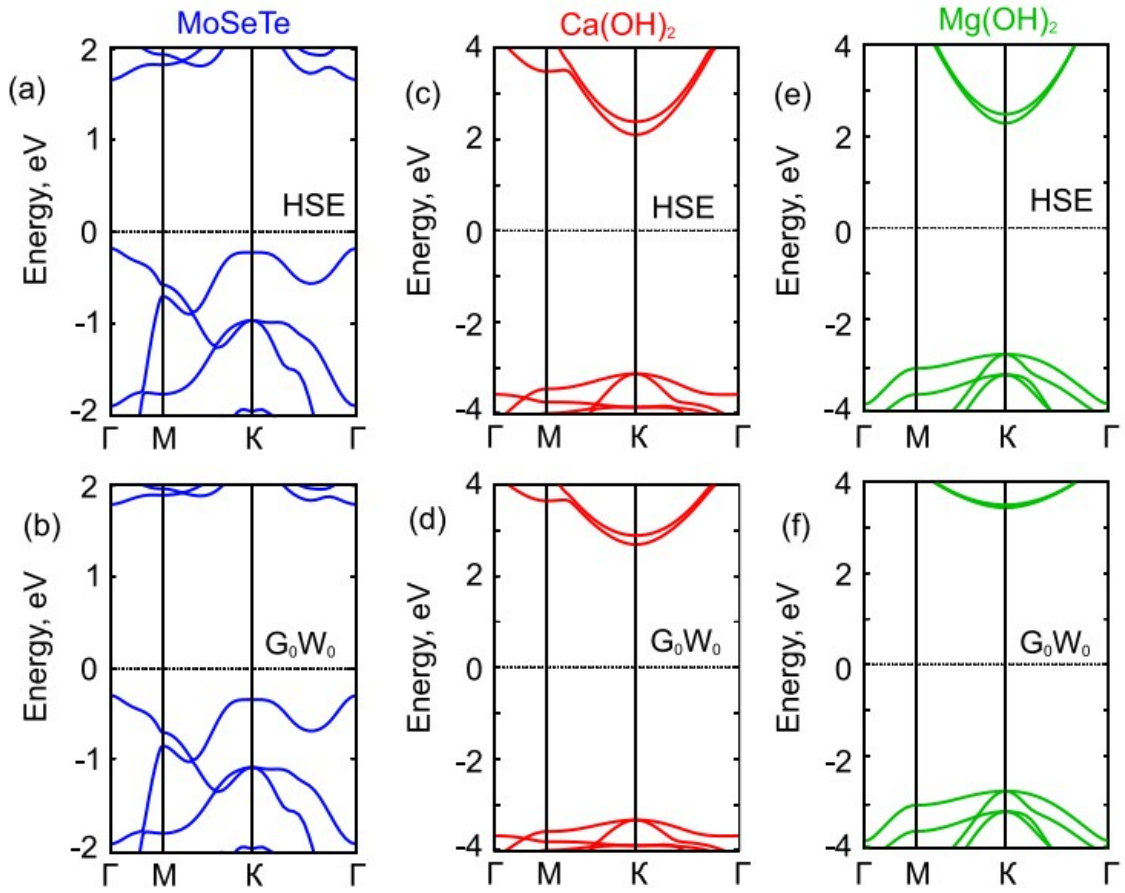

Fig. S1. Band structures of (a, b) Janus-MoSeTe, (c, d) $Ca(OH)_2$ and (e, f) $Mg(OH)_2$ monolayers at the equilibrium state calculated by (HSE, G_0W_0) methods, respectively.

To obtain more accurate band structure, we apply the HSE06 and G_0W_0 methods. The calculated band structures of Janus-MoSeTe, $Ca(OH)_2$ and $Mg(OH)_2$ monolayers at the equilibrium state with HSE06 and G_0W_0 methods are depicted in Fig. S1. The band gaps of the Janus-MoSeTe, $Ca(OH)_2$ and $Mg(OH)_2$ monolayers given by PBE/HSE06/G_0W_0 methods are calculated to be 1.27/1.71/2.14 eV, 3.68/5.18/5.86 eV, and 3.25/4.75/6.51 eV, respectively. However, despite the band gaps, the dispersions of the band structures with three methods exhibit the similar tendency in both valence band maximum and conduction band minimum. Thus, the PBE functional is used here and reliable results can be expected. In addition, both HSE06 and G_0W_0 calculations are enormously computationally intensive and demanding as compared to PBE method. Therefore, the electronic properties of the MoSeTe/$X(OH)_2$ at the equilibrium state and under electric field have been computed using the PBE functional in our present study. Whereas, the optical properties of such heterostructures are obtained by solving the Bethe-Salpeter equation (BSE) on top of single-shot G_0W_0 calculations, that include screening and excitonic effects.

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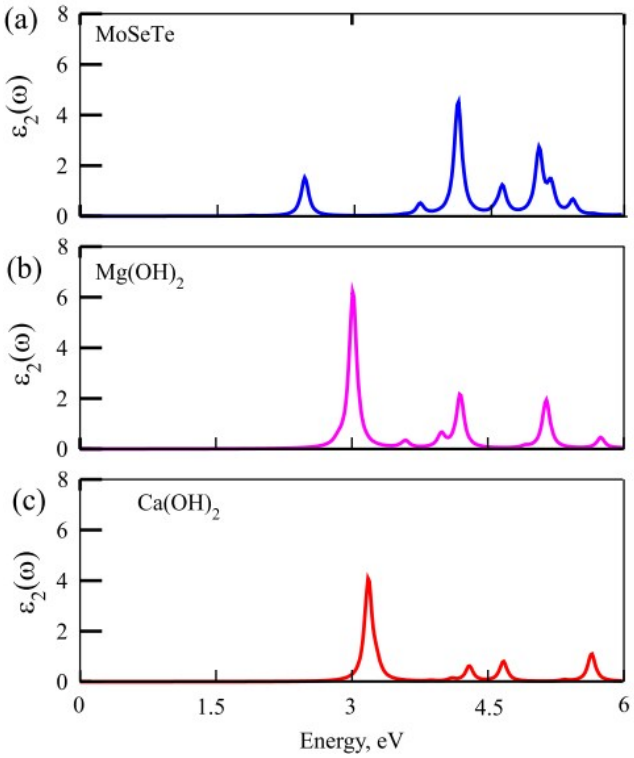

Fig. S2. Imaginary part of the dielectric function of the isolated (a) MoSeTe, (b) $Mg(OH)_2$ and (c) $Ca(OH)_2$ monolayers.

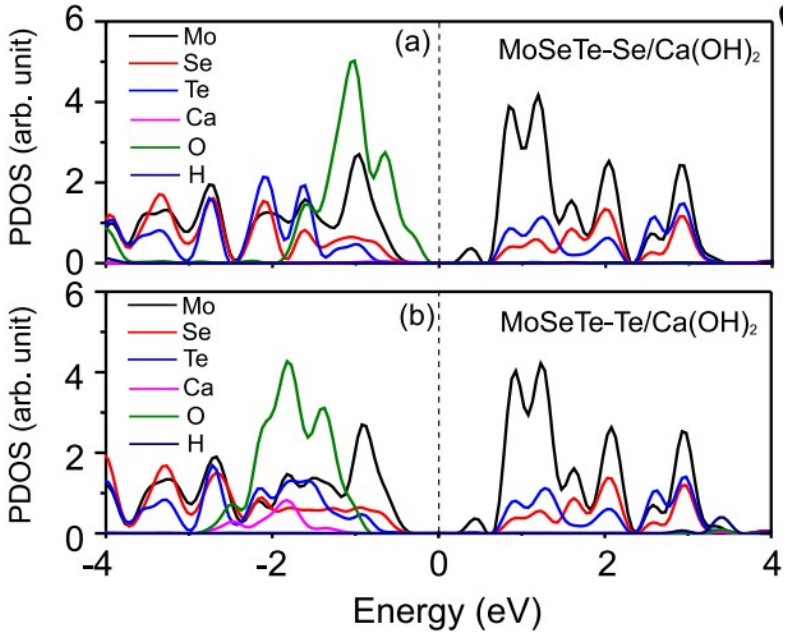

Fig. S3. Partial density states (PDOS) of the MoSeTe-Se/$Ca(OH)_2$ and (b) MoSeTe-Te/$Ca(OH)_2$ heterostructures. The Fermi level is set to be zero and marked by the dashed line.

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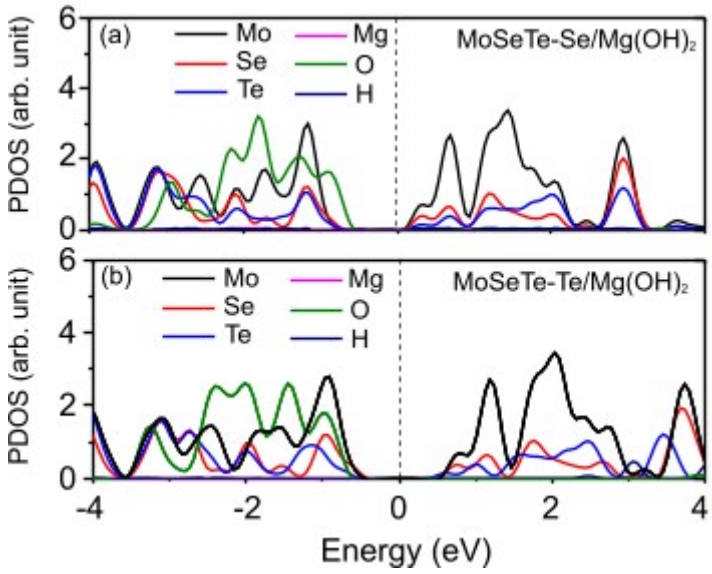

Fig. S4. Partial density states (PDOS) of the MoSeTe-Se/$Mg(OH)_2$ and (b) MoSeTe-Te/$Mg(OH)_2$ heterostructures. The Fermi level is set to be zero and marked by the dashed line.

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