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Band alignment of Zr2CO2/MoS2 heterostructure under electric field

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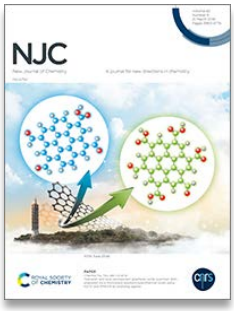

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Band alignment of Zr_2CO_2/MoS_2 heterostructure under electric field

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1. Cohesive energies of Ti_2CO_2/MoS_2 heterostructures

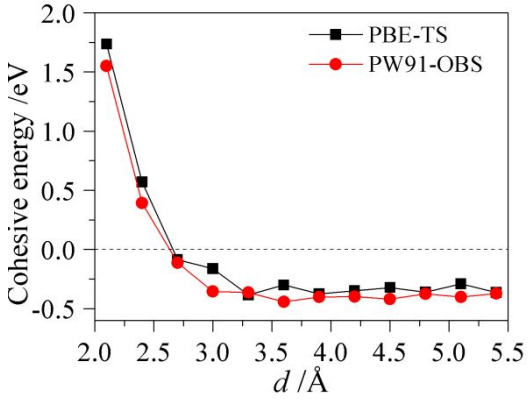

Figure S1. Cohesive energies of Ti_2CO_2/MoS_2 heterostructures with different interlayer spacing using PBE-TS and PW91-OBS.

2. Energy band structure of MoS_2

The state-of-the-art hybrid DFT approach based on the Heyd-Scuseria-Ernzerhof functional (HSE06) was used to calculate the electronic structures of MoS_2 after geometric optimization. In the default hybrid functional HSE06, the screening parameter μ and the mixing parameter α are set as 0.21 $Å^{-1}$ and 0.25, respectively. And norm-conserving pseudopotentials were used for all-electron HSE06 calculations. The calculated band gap of monolayer MoS_2 is 2.29 eV at the high symmetry K point, which is slightly larger than the experimental band gap of about 1.80 eV.

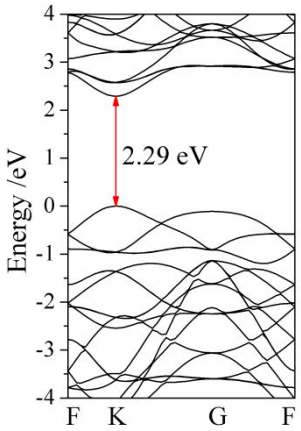

Figure S2. Energy band structure of monolayer MoS_2 using hybrid functional HSE06.

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(1) J. Heyd, G. E. Scuseria, M. Ernzerhof, Hybrid Functionals Based on a Screened Coulomb Potential. *J. Chem. Phys.* 2003, **118**, 8207–8215.

(2) J. S. Lin, A. Qteish, M. C. Payne, V. Heine, Optimized and Transferable Nonlocal Separable Ab Initio Pseudopotentials. *Phys. Rev. B* 1993, **47**, 4174–4180.

(3) K. F. Mak, C. Lee, J. Hone, J. Shan, T. F. Heinz, Atomically Thin MoS_2: A New Direct-Gap Semiconductor. *Phys. Rev. Lett.* 2010, **105**, 2–5.

3. Definition of charge density difference

The charge density difference is defined as

$$\Delta\rho = \rho_{Zr_2CO_2/MoS_2} - \rho_{Zr_2CO_2} - \rho_{MoS_2} \quad \text{(S1)}$$

where $\rho_{Zr_2CO_2/MoS_2}$, $\rho_{Zr_2CO_2}$ and ρ_{MoS_2} represent the charge densities of Zr_2CO_2/MoS_2 heterostructures, isolated Zr_2CO_2 and MoS_2 layers, respectively. Namely, the charge density difference can be obtained by subtracting the electronic charge density of Zr_2CO_2/MoS_2 heterostructure from those of the corresponding isolated Zr_2CO_2 and MoS_2 layers, respectively.

4. The stereo charge density differences of Zr_2CO_2/MoS_2 heterostructures

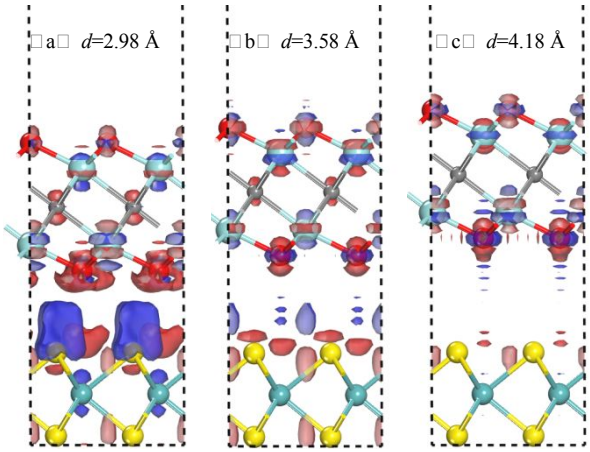

Figure S3. The stereo charge density differences of Zr_2CO_2/MoS_2 heterostructures for three different interlayer spacings using PBE-TS, in which red and blue isosurfaces denote charge augmentation and diminution in the space, respectively. The isovalue of 0.0005 e/Å^{-3} is chosen to plot the isosurface.

5. Definition of CB and VB edge potentials

The band edge energies of CB and VB of MoS_2 and Zr_2CO_2 from electronegativity and BG of semiconductor are defined as

$$E_{VB} = \chi + 0.5E_g + E_e \quad \text{(S2)}$$

$$E_{CB} = E_{VB} - E_g \quad \text{(S3)}$$

where χ is the average absolute electronegativity of semiconductor. E_e is the energy of free electron on the hydrogen scale (4.5 eV). And E_{CB}, E_{VB}, E_g are the band edge energies of the CB, VB and BG of semiconductor, respectively.

6. Optical absorption coefficient spectra

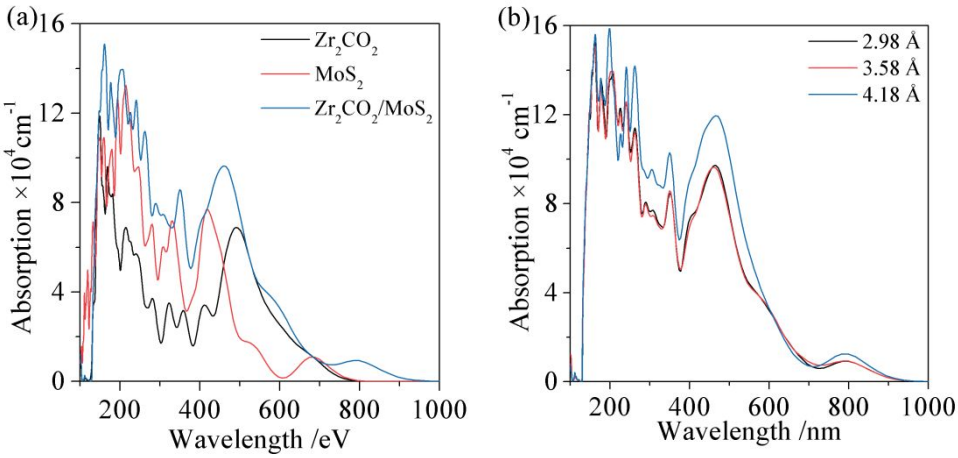

Fig. S4. Calculated total optical absorption coefficient spectra of (a) isolated system and (b) Zr_2CO_2/MoS_2 heterostructure with different interlayer spacings using PBE-TS.

7. Energy band structures of Zr_2CO_2/MoS_2 heterostructures under the E_{field}

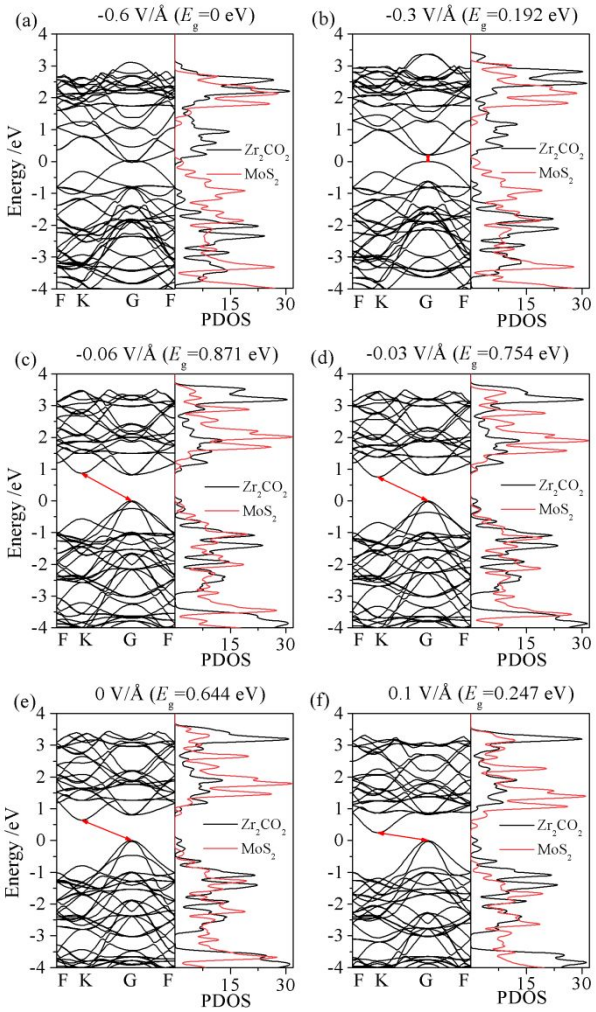

Figure S5. Energy band structures of Zr_2CO_2/MoS_2 heterostructures with different E_{field}.