

Supporting Information

for

Electronic Structure and Photocatalytic Band Offset of Few-layer GeP₂

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Table S1. Lattice constants and relative stabilities of monolayers of other less stable GeP₂ phases predicted by CALYPSO. Note that all of them adopt rectangular 2D crystals. Distances and energies are in units of Å and eV/cell, respectively.

Phase	E _{rel} ^a	(<i>a</i> , <i>b</i>) ^b
O-2	0.014	(6.29,3.53)
O-3	0.565	(7.09,3.55)
O-4	0.708	(6.42,4.00)

^aRelative energy with respect to the penta-GeP₂ monolayer.

^bOptimized lattice constants based on the optB88-vdW .

Figure S1. Chemical structures of the other less stable GeP_2 monolayers predicted by CALYPSO: O-2 (a), O-3 (b), and O-4 (c) shown in two different views. Purple and brown colors represent germanium (Ge) and phosphorus (P) atoms, respectively.

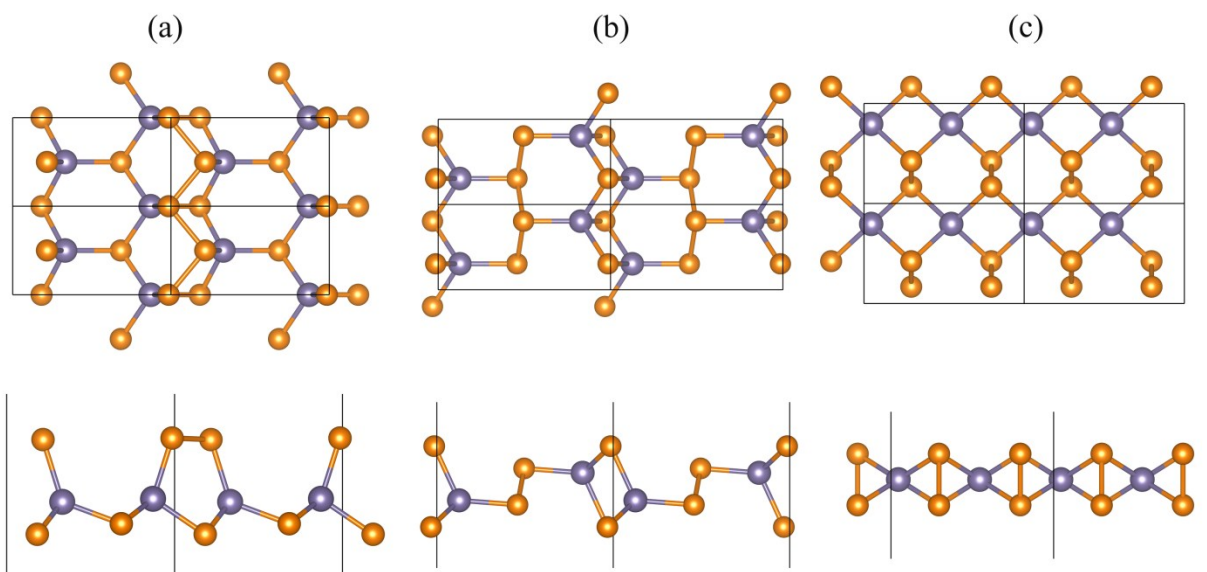
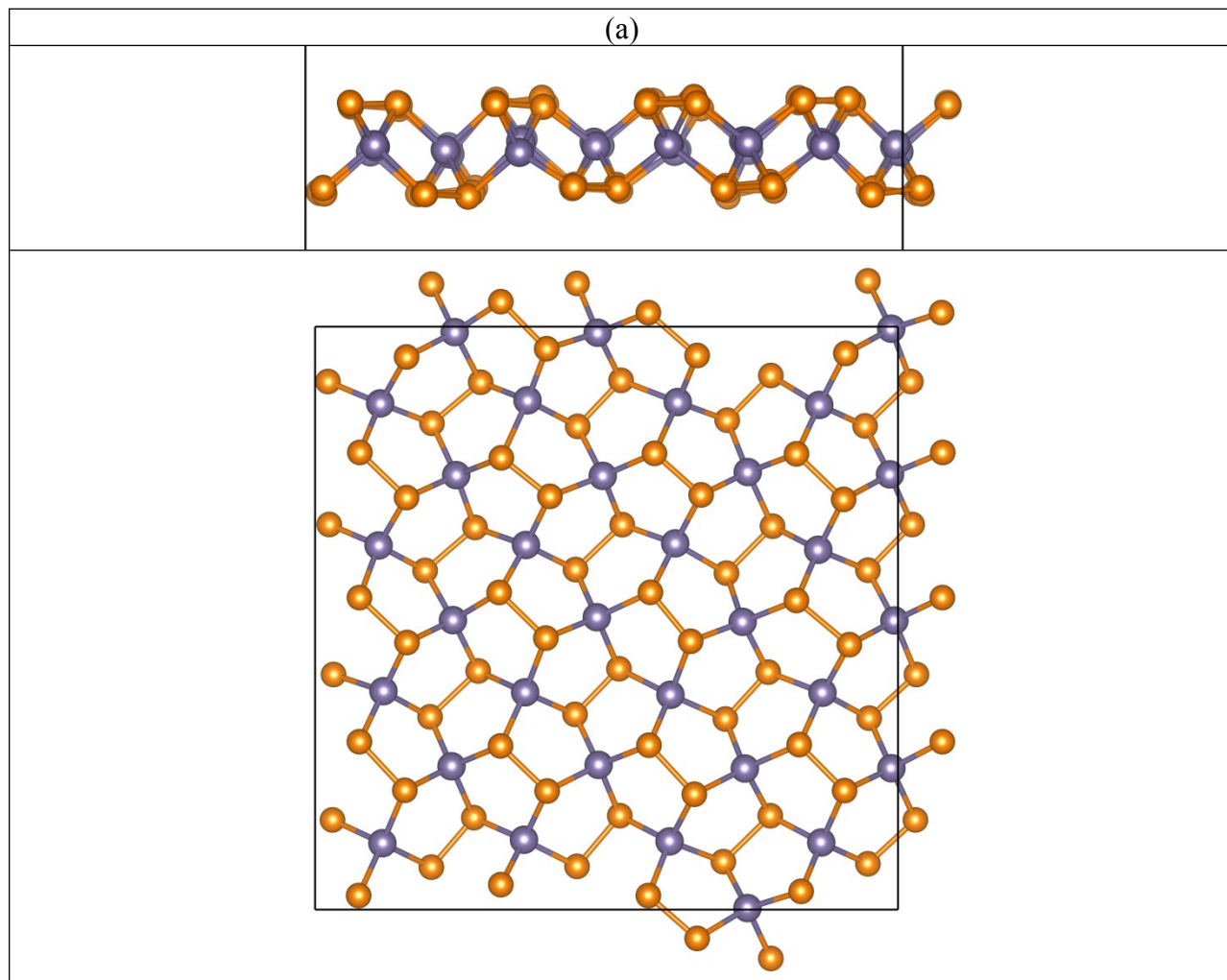
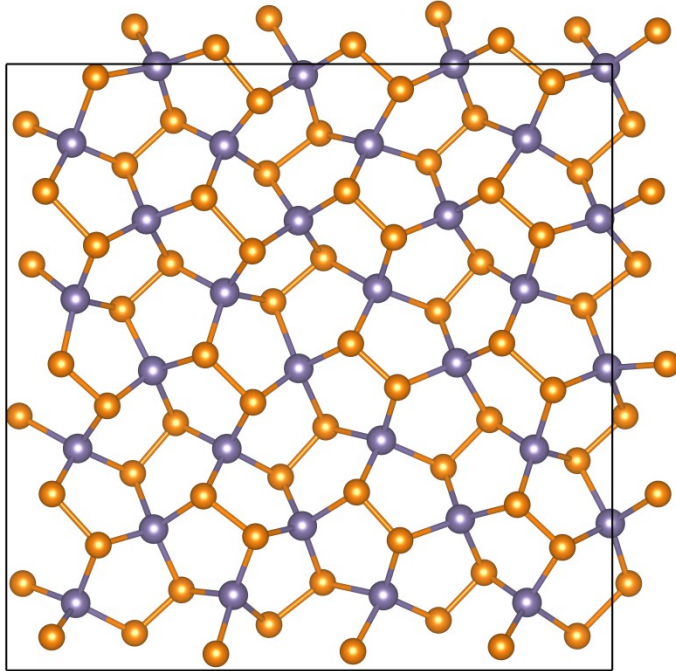
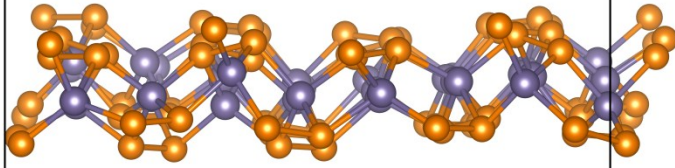


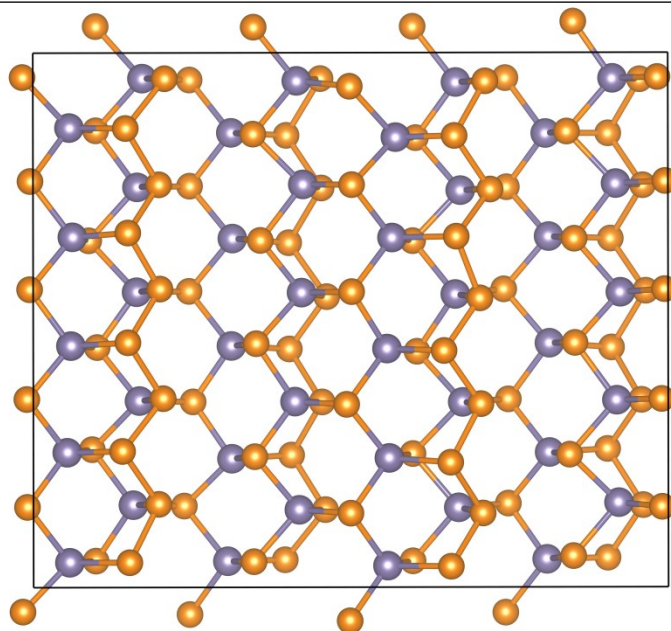
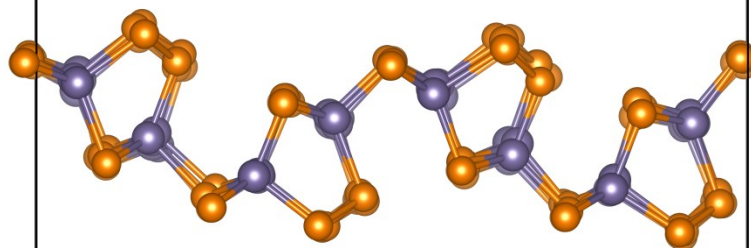
Figure S2. Chemical structures of penta-GeP₂ (a, b) and O-GeP₂ (c,d) at 300 K (a,c) and 700 K (b,d) after 4 ps of *ab initio* MD simulation. Purple and brown colors represent germanium (Ge) and phosphorus (P) atoms, respectively.



(b)



(c)



(d)

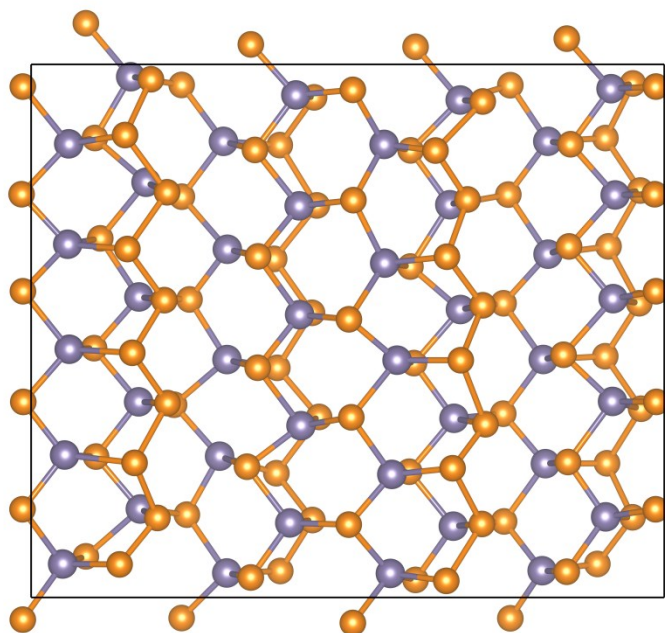
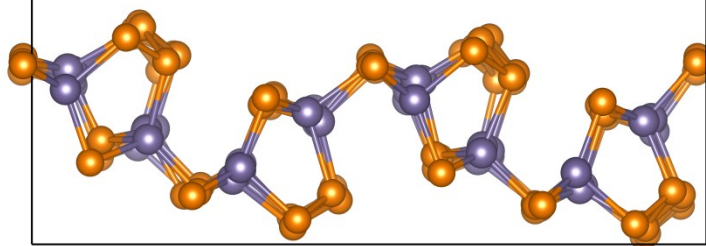


Figure S3. Chemical structures of the penta-GeP₂ bilayer in various stacking patterns: AA, AB, AB', and AA' in two different views. Also shown are those of the O-GeP₂ bilayer in stacking patterns BB and AA. Purple and brown colors represent germanium (Ge) and phosphorus (P) atoms, respectively. For clarity, atoms belonging to different layers are distinguished by different colors.

