

**Using van der Waals heterostructures based on two-dimensional  
blue phosphorus and XC (X = Ge, Si) for water-splitting  
photocatalysis: A first-principles study**

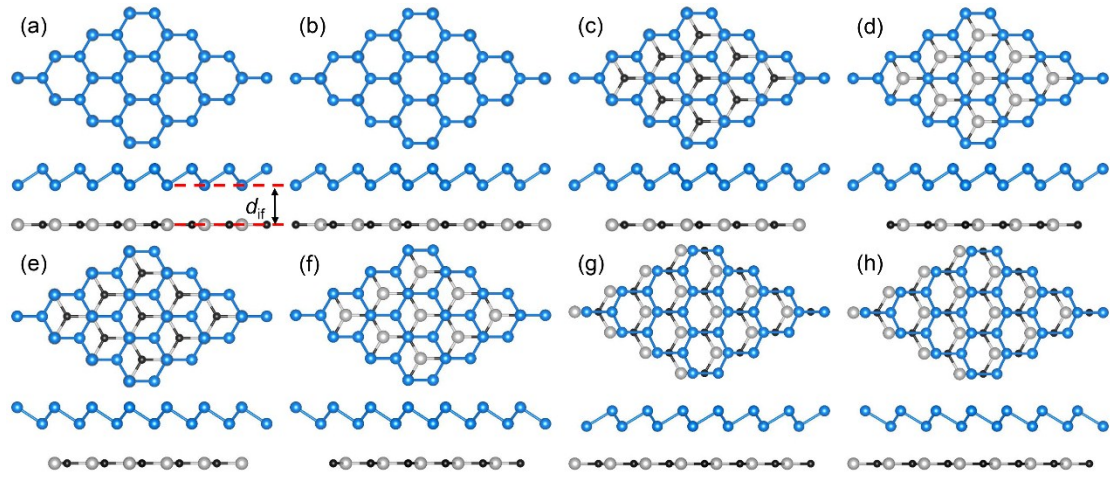
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**Fig. S1** Top and side views of BlueP/XC ( $X = \text{Ge}, \text{Si}$ ) heterostructure for different stacking illustrations: (a) A-stacking, (b) B-stacking, (c) C-stacking, (d) D-stacking, (d) D-stacking, (e) E-stacking, (f) F-stacking, (g) G-stacking, (h) H-stacking. The blue, black and gray spheres represent the P, C and Ge (Si) atoms, respectively.