Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Type-II 2D AgBr/SiH van der Waals Heterostructures with Tunable Band Edge Position and Enhanced Optical Absorption Coefficient for Photocatalytic Water Splitting

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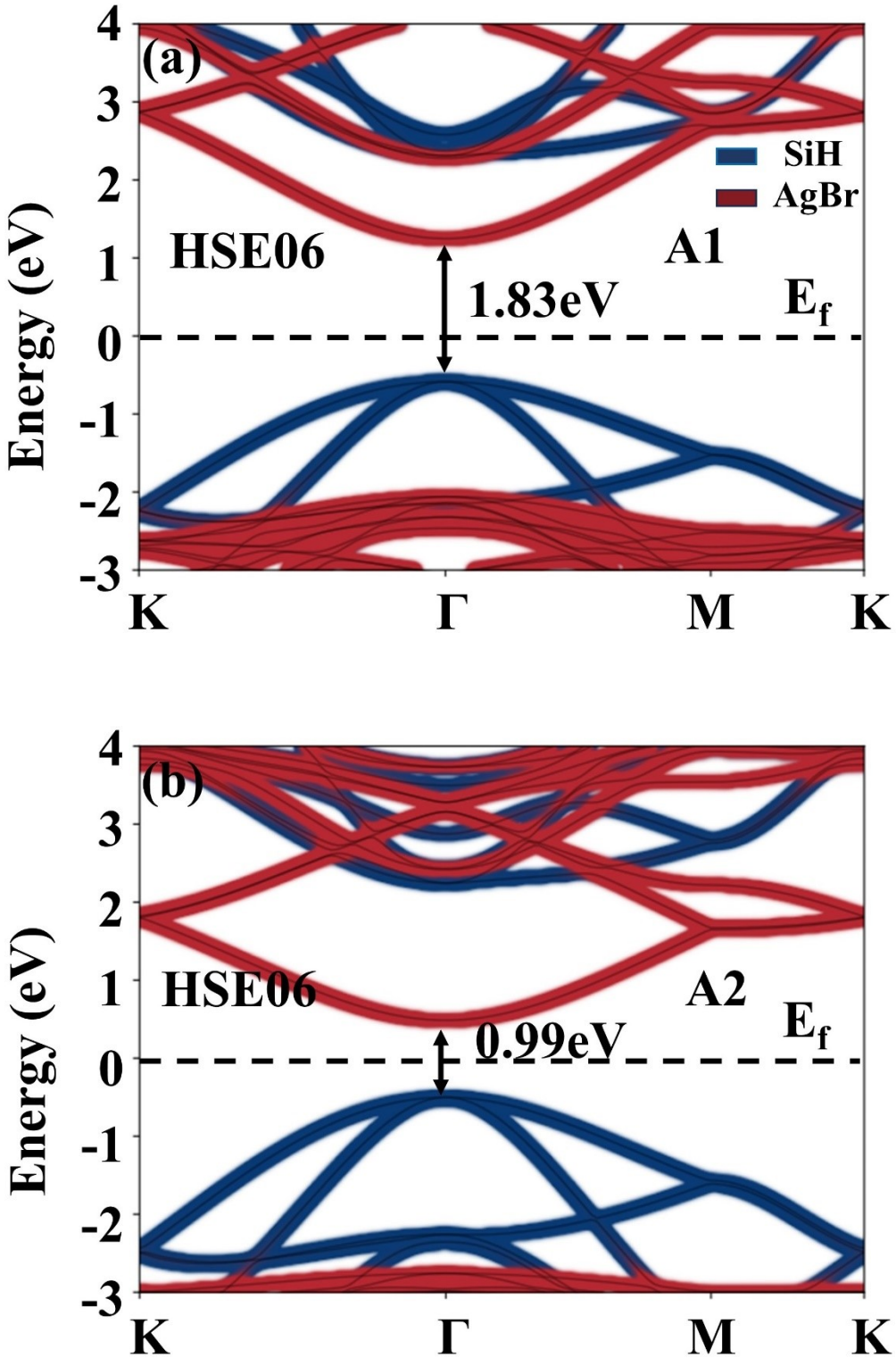

(a)
SiH
AgBr
HSE06
A1
1.83eV
E_f
Energy (eV)
4
3
2
1
0
-1
-2
-3
K
Γ
M
K
(b)
HSE06
A2
0.99eV
E_f
Energy (eV)
4
3
2
1
0
-1
-2
-3
K
Γ
M
K

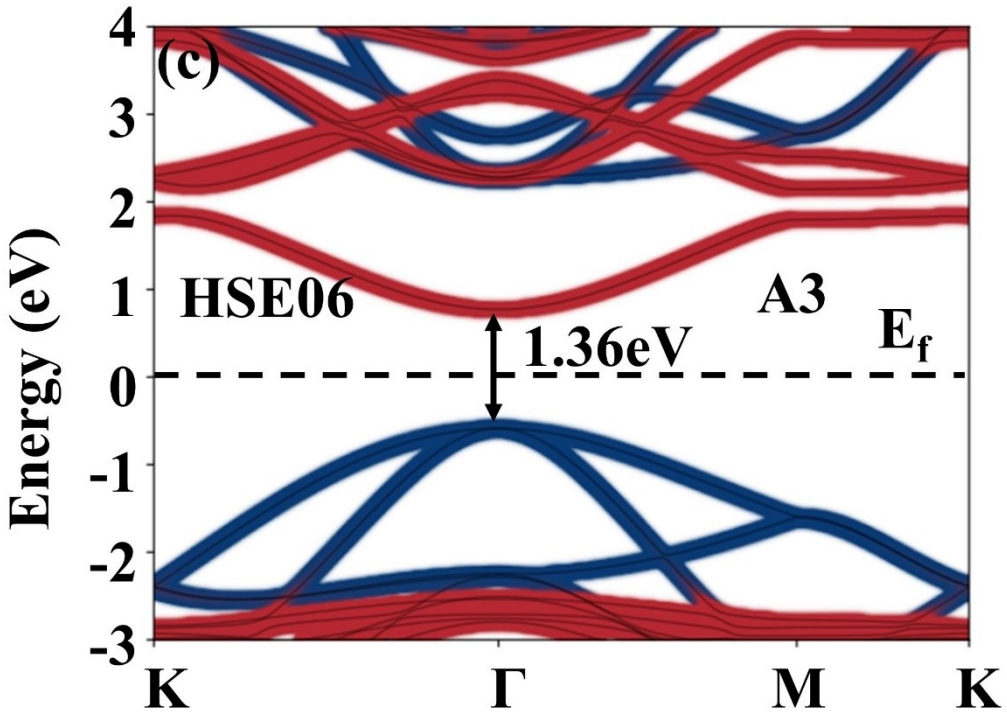
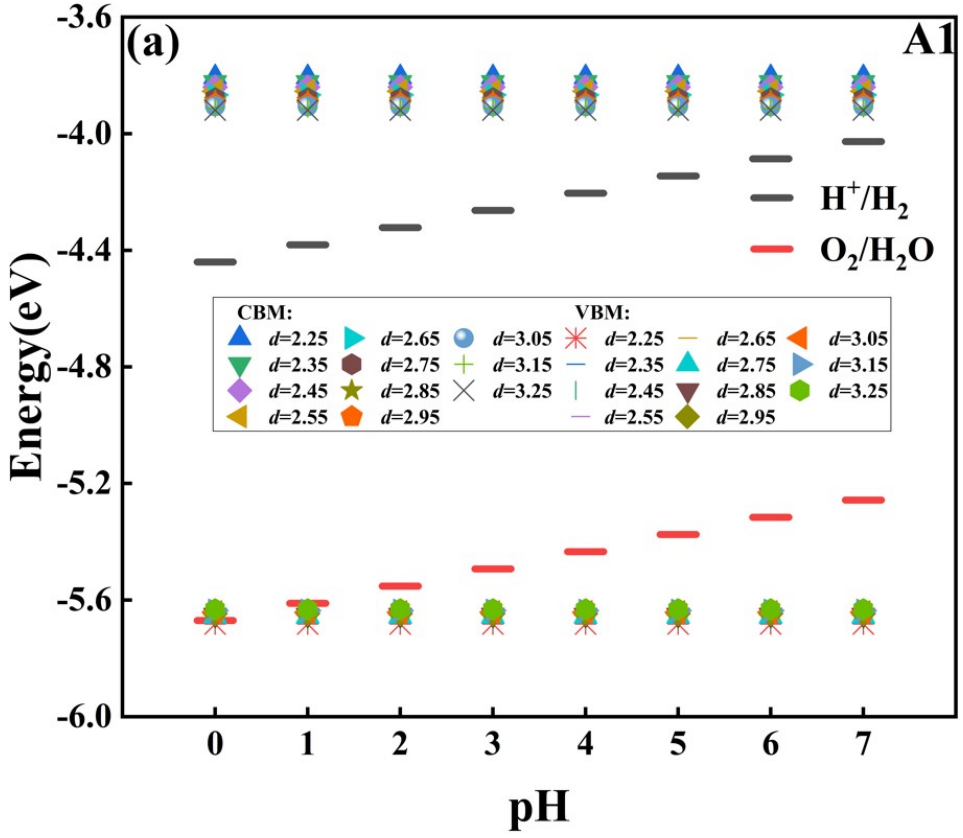


Fig. S1. The projected band structure of (a)A1, (b)A2, and (c)A3 configurations using the HSE06 functional.



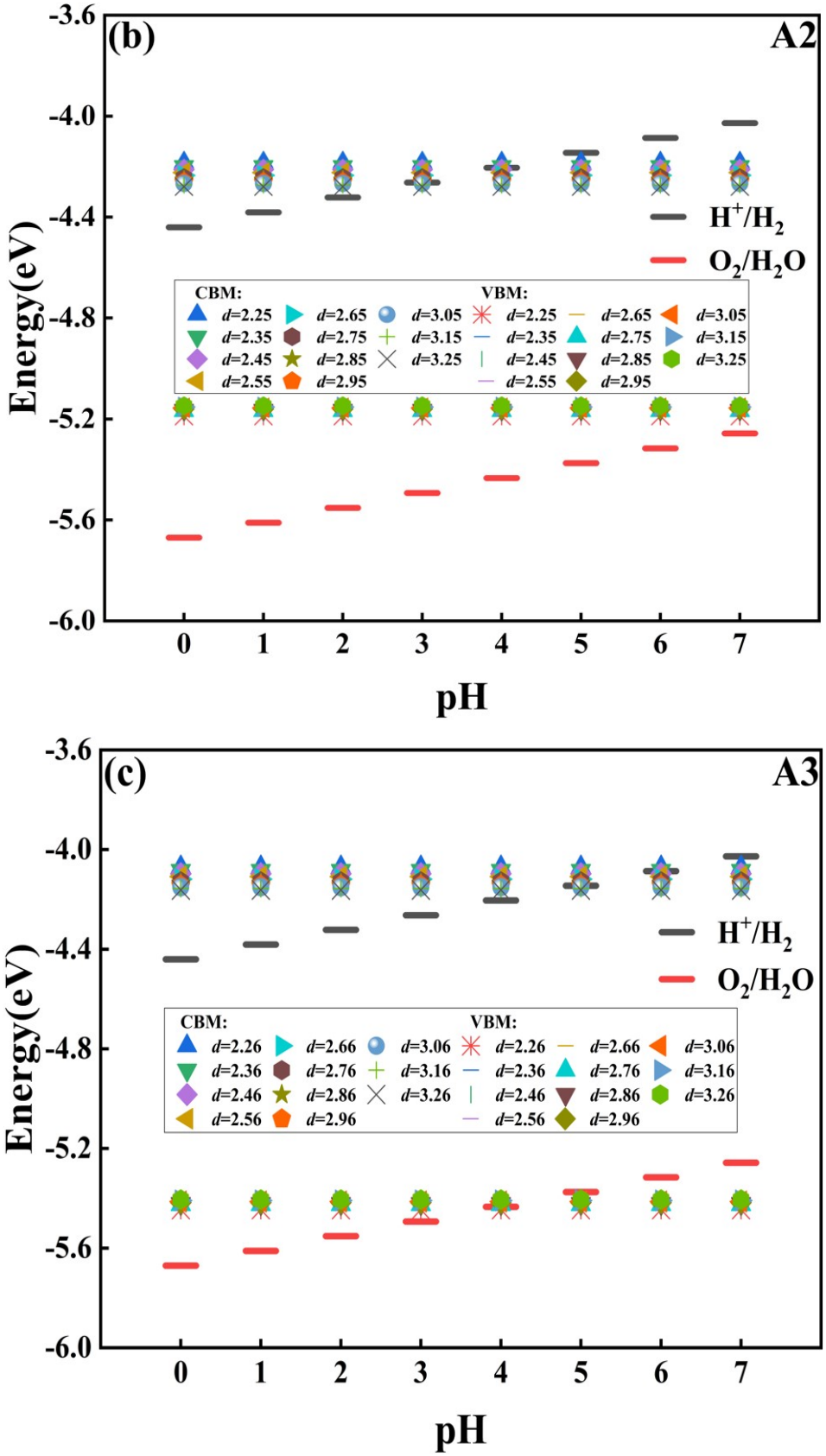


Fig. S2. The band edge position of (a) A1, (b) A2, and (c) A3 configurations with changing interlayer distance *d* from 2.25 (2.26) Å to 3.25(3.26) Å in the pH range of 0 to 7.