Supplementary Material

of

Tunable electronic band structure of $AlP_3/Cs_3Bi_2I_6Cl_3$ van der Waals heterostructure induced by electric field: a first-principles study

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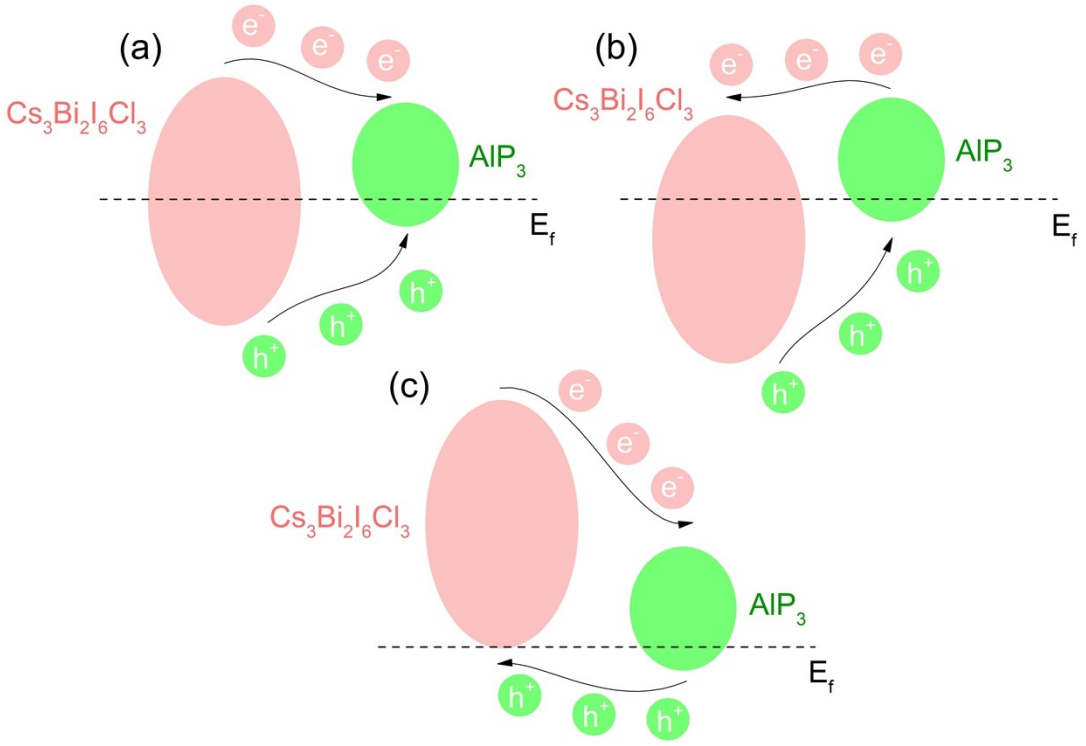

Figure S1 Schematic illustration of the band alignment of $AlP_3/Cs_3Bi_2I_6Cl_3$ vdWH under an external electric field of (a) 0 V/Å, (b) 0.1 V/Å and (c) -0.2V/Å, respectively

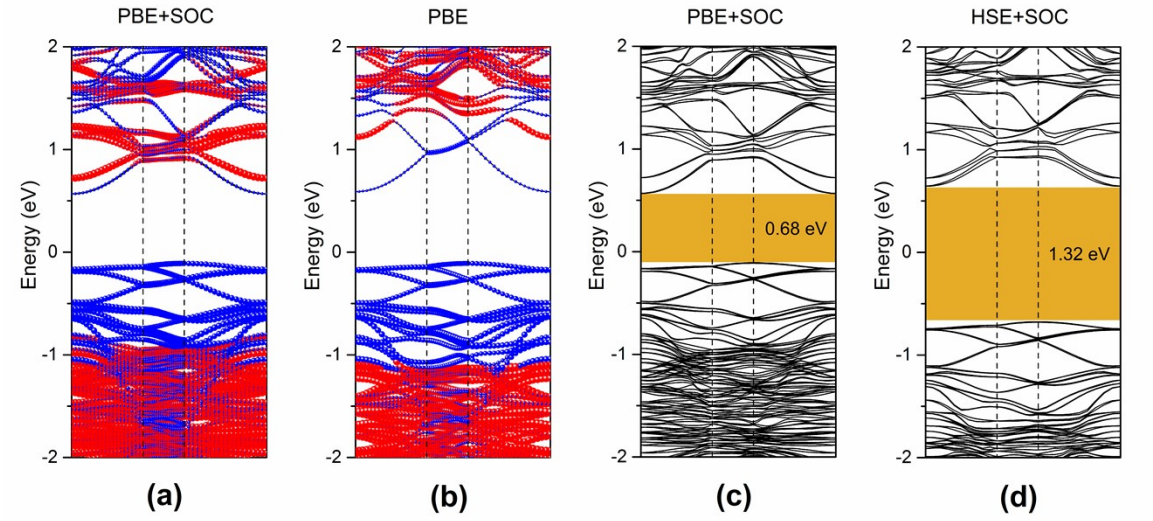

Figure S2 (a) The projected band structure of $AlP_3/Cs_3Bi_2I_6Cl_3$ vdWH calculated by PBE+SOC functional. (b) The projected band structure of $AlP_3/Cs_3Bi_2I_6Cl_3$ vdWH calculated by PBE functional. (c) The electronic band structure of $AlP_3/Cs_3Bi_2I_6Cl_3$ vdWH calculated by PBE+SOC functional. (d) The electronic band structure of $AlP_3/Cs_3Bi_2I_6Cl_3$ vdWH calculated by HSE+SOC functional.

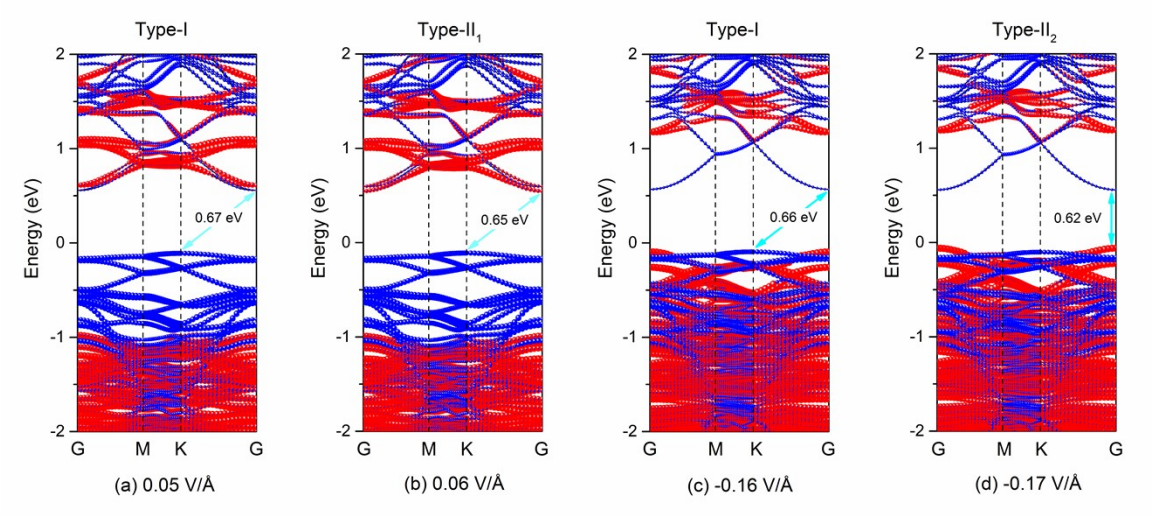

Figure S3. The electronic band structures under external electric fields of (a) 0.05 V/Å, (b) 0.06 V/Å, (c) -0.16 V/Å and (d) -0.17 V/Å for $AlP_3/Cs_3Bi_2I_6Cl_3$ vdWH. The Fermi level is set to zero.