SUPPLEMENTARY INFORMATION

Coexistence of spin valley coupled Dirac semimetal and robust quantum spin Hall state with significant Rashba spin splitting in halogenated BiAs film

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Figure S1: AIMD simulation of the energy variation of a d-ClBiAsI monolayer. Side view of the crystal structure after 3 picoseconds are shown in right panels.



Figure S2: (a) Orbital projected band structure at 0% with inclusion of SOC (b) spin-resolved band structure of d-ClBiAsI monolayer at 0%.



Figure S3: Electronic band structure of s-ClBiAsI monolayer (a) without SOC (b) with SOC.



Figure S4: (a) phonon dispersion curves of AA stacked d-ClBiAsI and (b) AIMD simulation of bilayer d-ClBiAsI AT 300k.



Figure S5: crystal structure of AB stacked d-ClBiAsI (left panel) and electronic band structure of bilayer d-ClBiAsI (a) without SOC and (b) with SOC.



Figure S6: crystal structure of AA' stacked d-ClBiAsI (left panel) and electronic band structure of bilayer d-ClBiAsI (a) without SOC and (b) with SOC.



Figure S7: Electronic band structure at 8% strain using HSE06 functional of (a) d-ClBiAsI monolayer and (b) AA- stack bilayer d-ClBiAsI