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Supporting Information For

Energetic and Electronic Properties of $CsPbBr_3$ Surfaces: A First-principles Study

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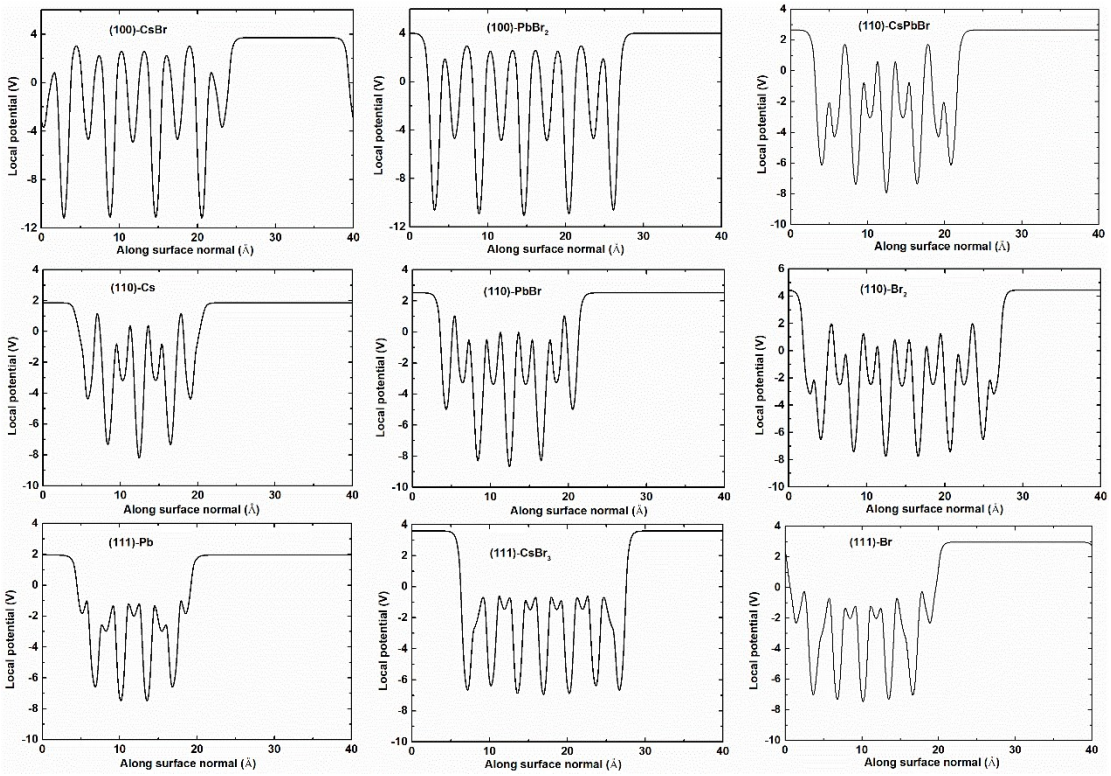

Fig. S1 Calculated planar-averaged local potential for all surfaces.

Table S1 Calculated formation energies (ΔH, eV) of CsBr, $PbBr_2$ and $CsPbBr_3$ with/without SOC. Formation energy of compounds is calculated with respect to element phases.

ΔH	CsBr	$PbBr_2$	$CsPbBr_3$
Without SOC	−3. 789	−3. 111	−7. 020
With SOC	−3. 787	−2. 926	−6. 860

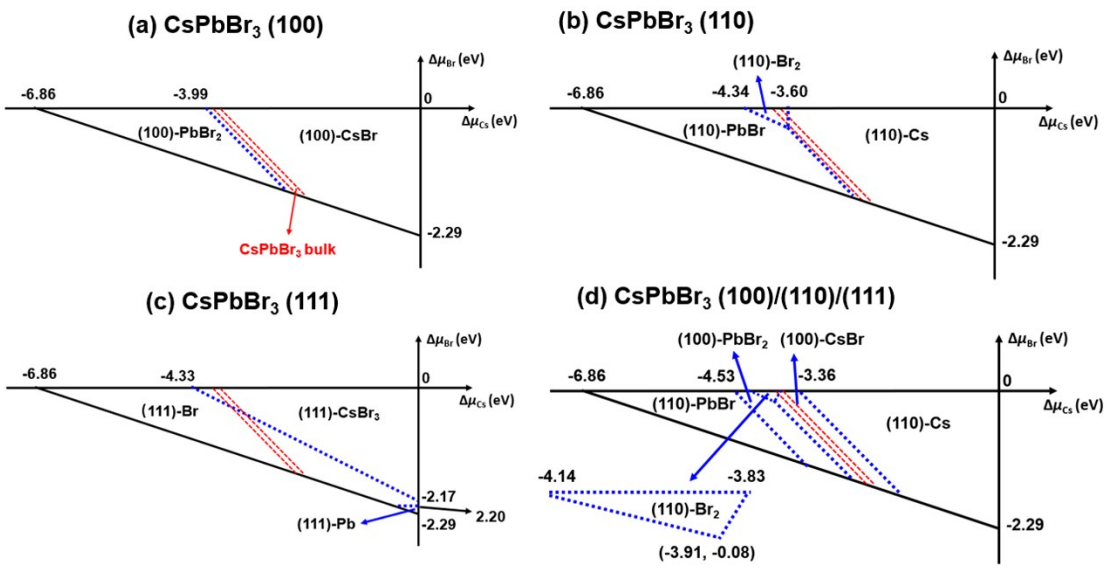

Fig. S2 PBEsol calculated phase diagrams of $CsPbBr_3$ (100), (110) and (111) surfaces with spin-orbital coupling (SOC) considered (PBEsol+SOC). The inclusion of SOC only induces minor shift of phase boundaries (small changes of numbers on chemical potential axes in comparison with PBEsol results in main text) and does not influence the order of the stability of the surfaces. We note that (111)-Pb only appears at very special condition of Br-poor and Cs-rich for (111) surfaces in SOC case.

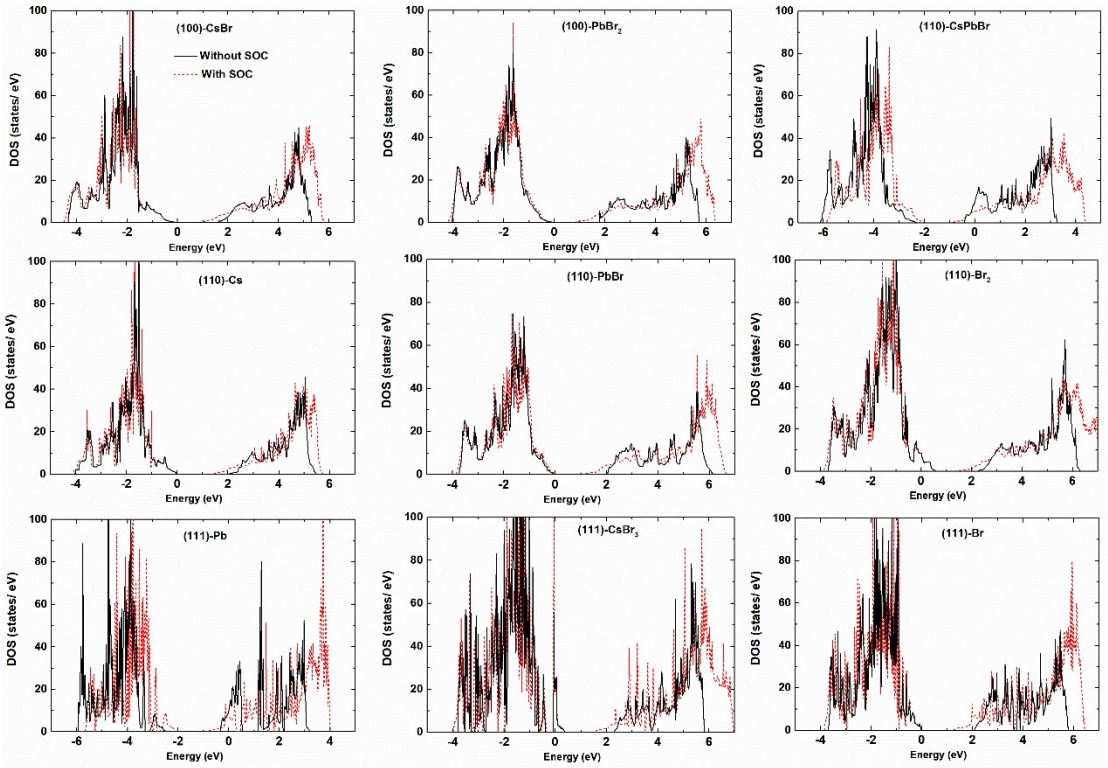

Fig. S3 PBEsol calculated density of states (DOS, states/eV) with/without SOC considered.

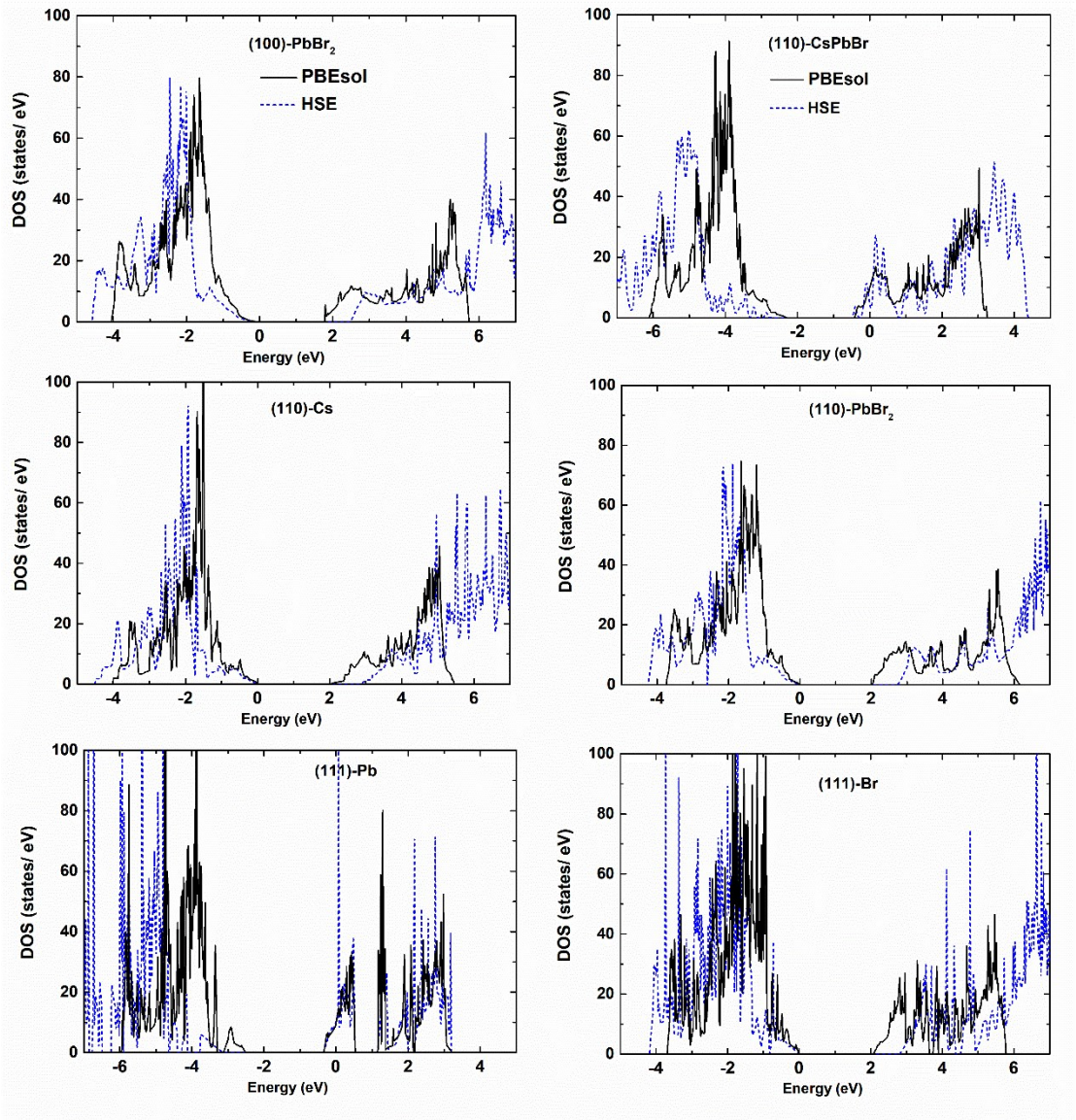

Fig. S4 PBEsol calculated DOS in comparison with HSE06 results. HSE06 is mixed with 25% Hartree−Fock exchange potential.