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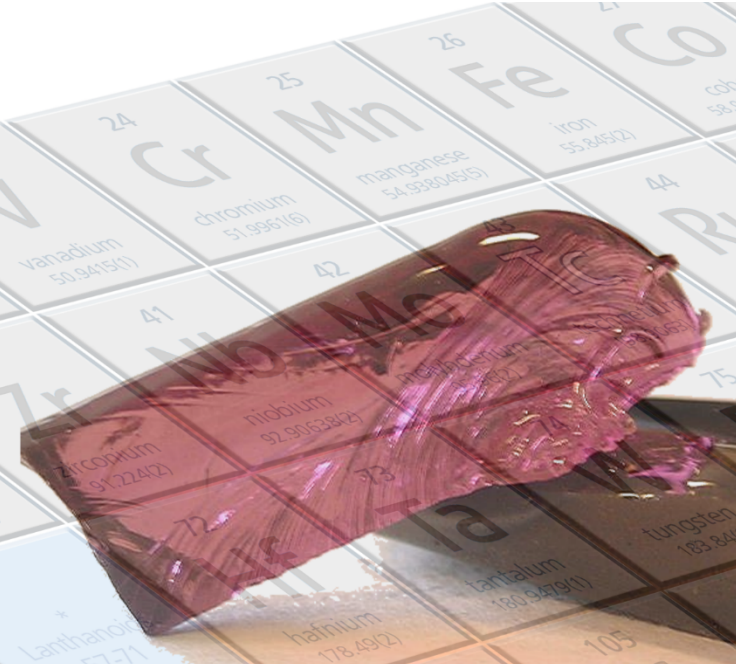
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ABINIT school : From January 30th, 2017 to February 3rd, 2017

Electronic properties of hybrid organic and inorganic perovskites

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In this poster we, first, present ABINIT based DFT results of the optoelectronic properties of $\text{CH}_3\text{NH}_3\text{PbI}_3$ and $\text{CH}_3\text{NH}_3\text{BCl}_3$ (B=Pb, Sn, Ge) hybrid organic-inorganic perovskites (HOP). For $\text{CH}_3\text{NH}_3\text{MCl}_3$ HOP, the pseudocubic high temperature reference HOP structure (Pm-3m) was used to compare spin-orbit coupling (SOC) induced effect due to the metal atom B.^[1-3]

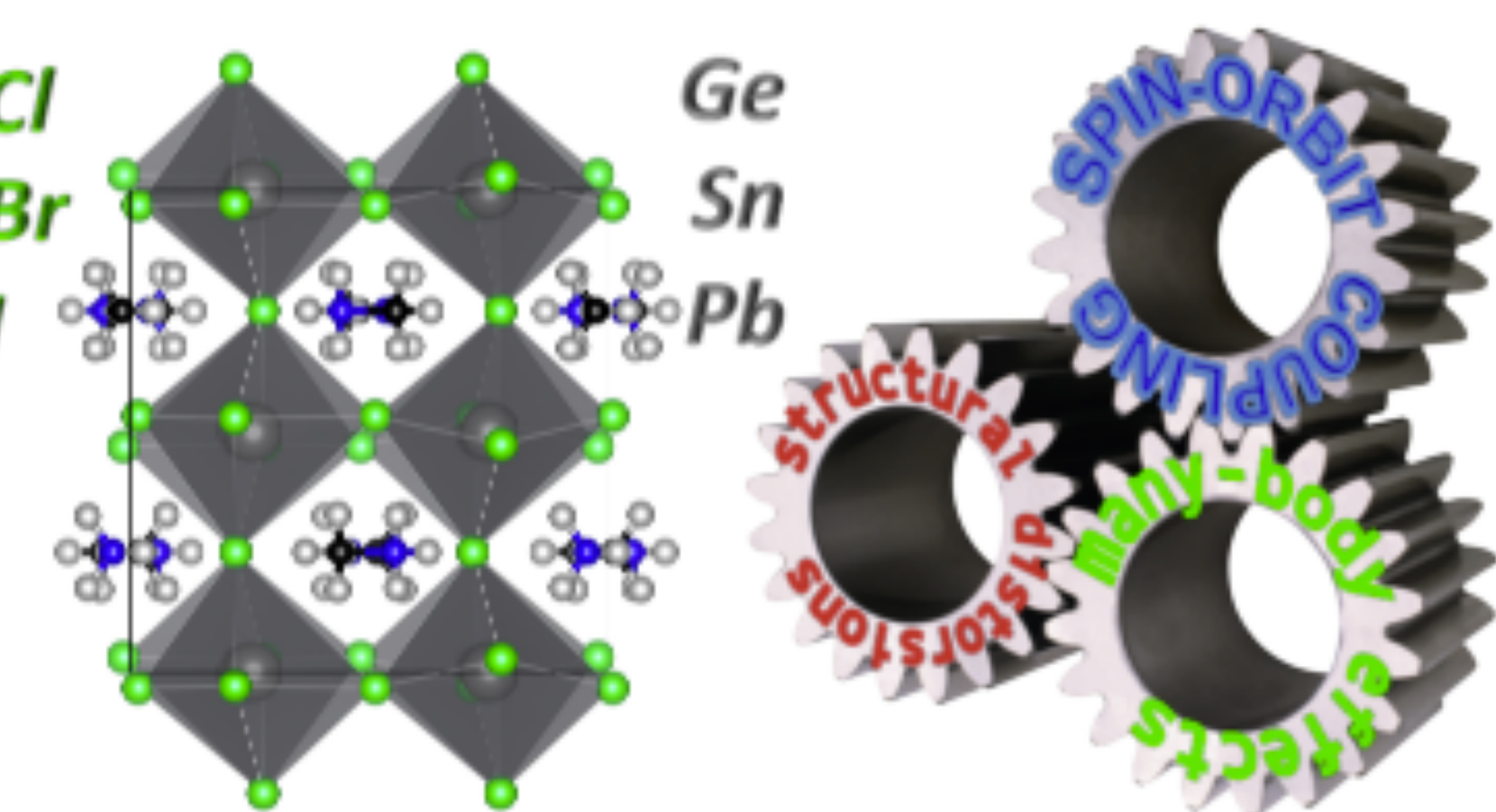
Next, we present 2D layered HOP which received a renewed interest in recent years due to increased stability under lighting conditions and resistance to humidity and moisture. Their electronic properties show their potential in photovoltaic and optoelectronic applications.^[4]

[1] J. Even, L. Pedesseau, J.-M. Jancu, C. Katan, *J. Phys. Chem. Lett.* 4, 2013

[2] C. Katan, L. Pedesseau, M. Kepenekian, A. Rolland, J. Even, *J. Mat. Chem. A*, 3, 2015

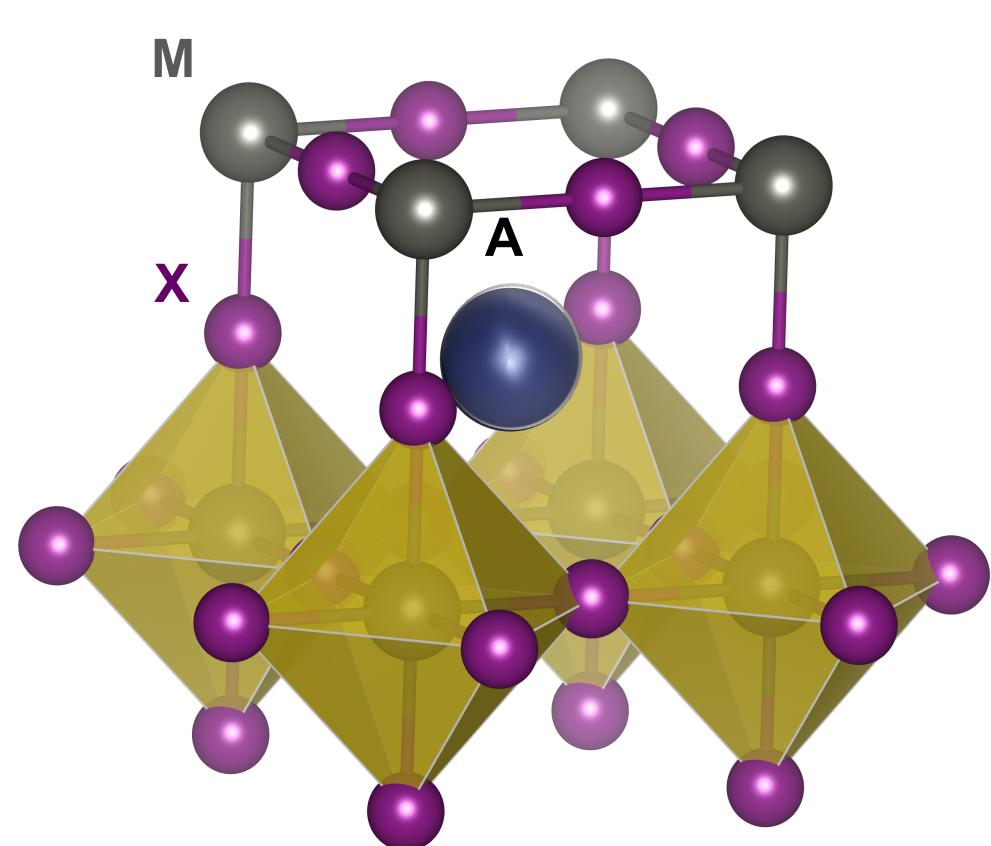
[3] J. Even, L. Pedesseau, J.-M. Jancu, C. Katan, *Phys. Status Solidi RRL*, 8, 2014

[4] J. Even, L. Pedesseau, M.A. Dupertuis, J.-M. Jancu, C. Katan, *PRB*, 86, 2012



3D hybrid organic-inorganic perovskites

Formula : ABX_3

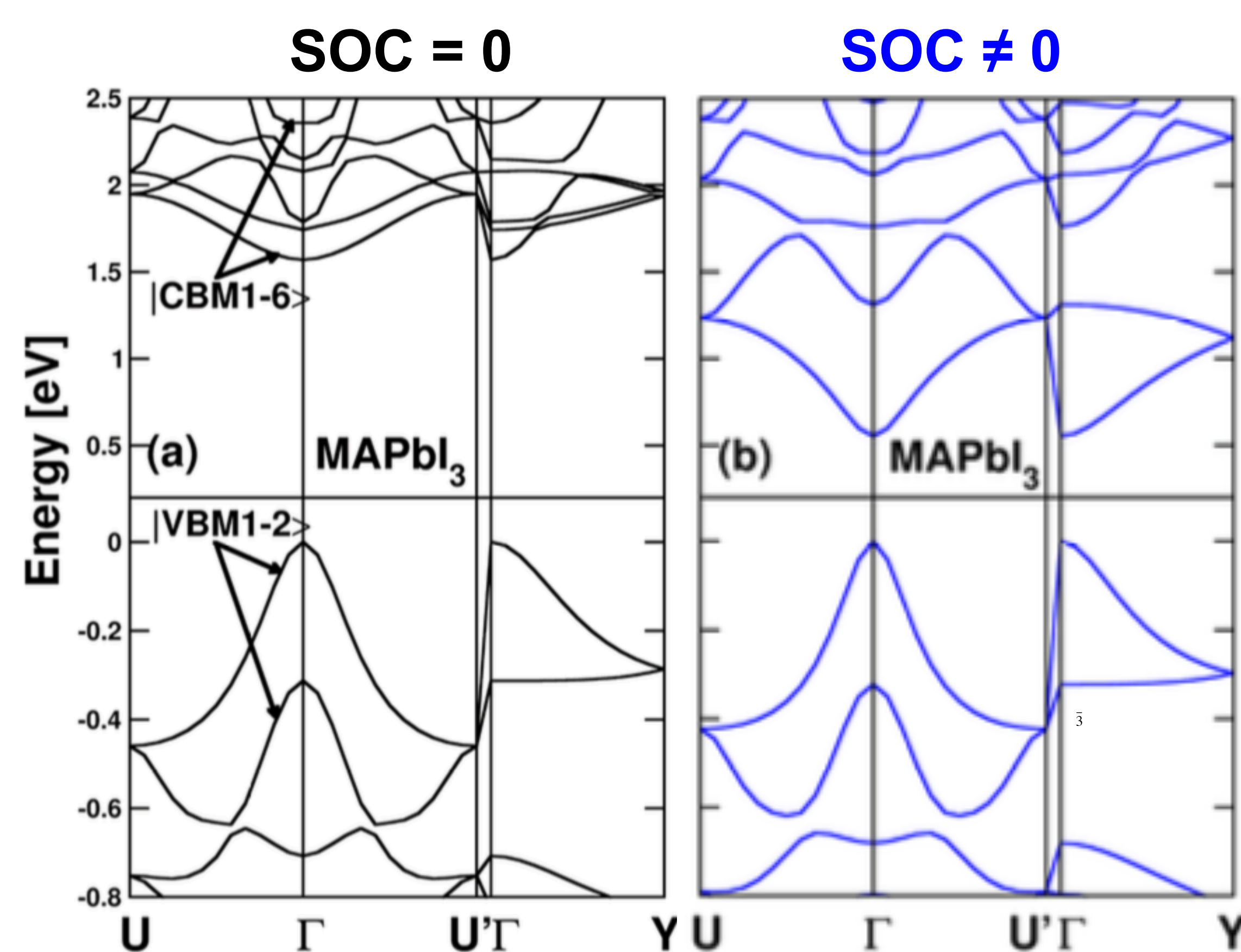


A : MA (CH_3NH_3); FA
($\text{HC}(\text{NH}_2)_2$); Cs; Rb

B : Inorganic cation
Pb; Sn; Ge; etc...

X : halogen (I, Br, Cl)

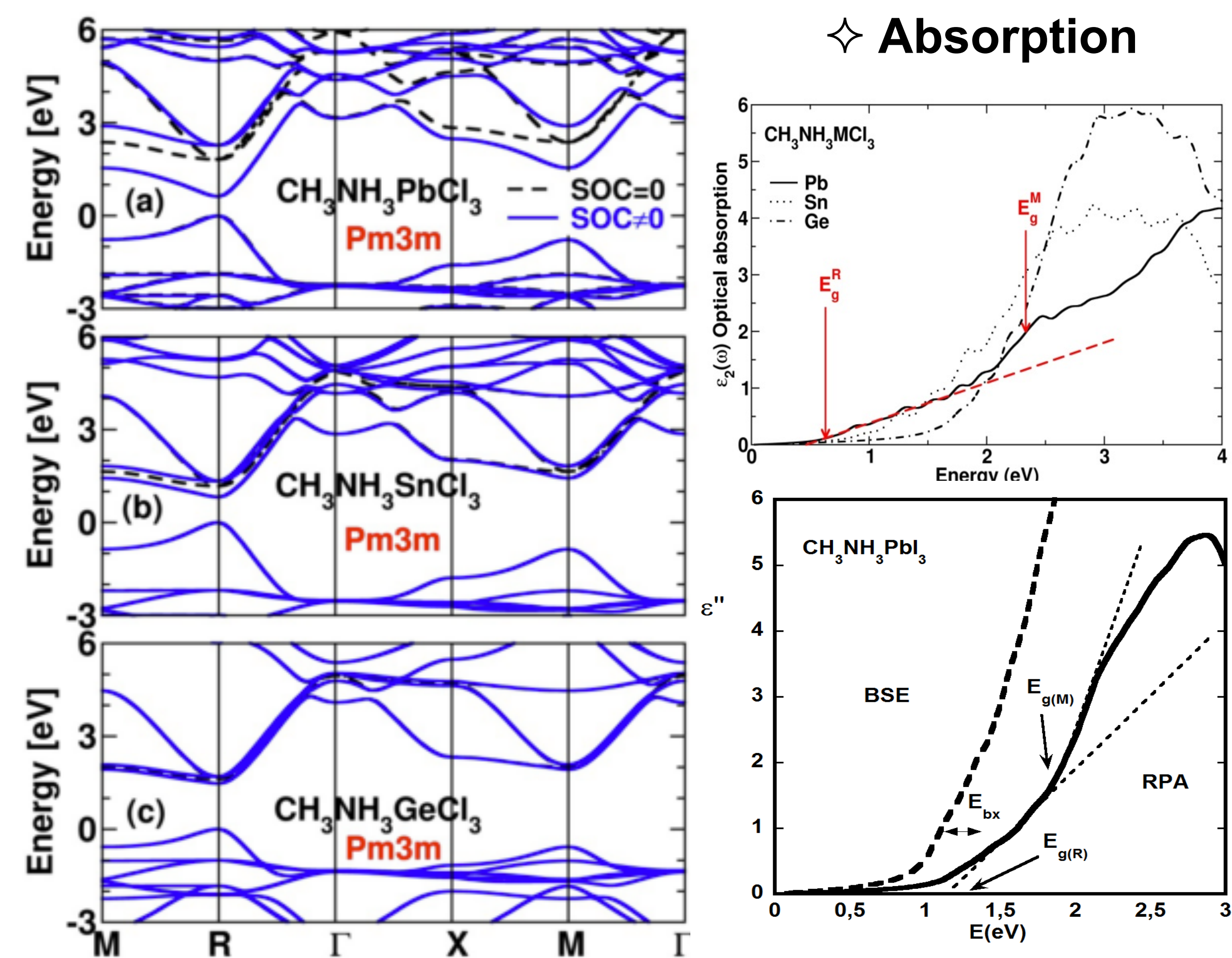
MAPbI_3 Pnma orthorhombic phase^[1]



✧ Band gap at Γ

✧ Importance of spin-orbit coupling effect

MABX_3 Pm-3m cubic phase^[2,3]



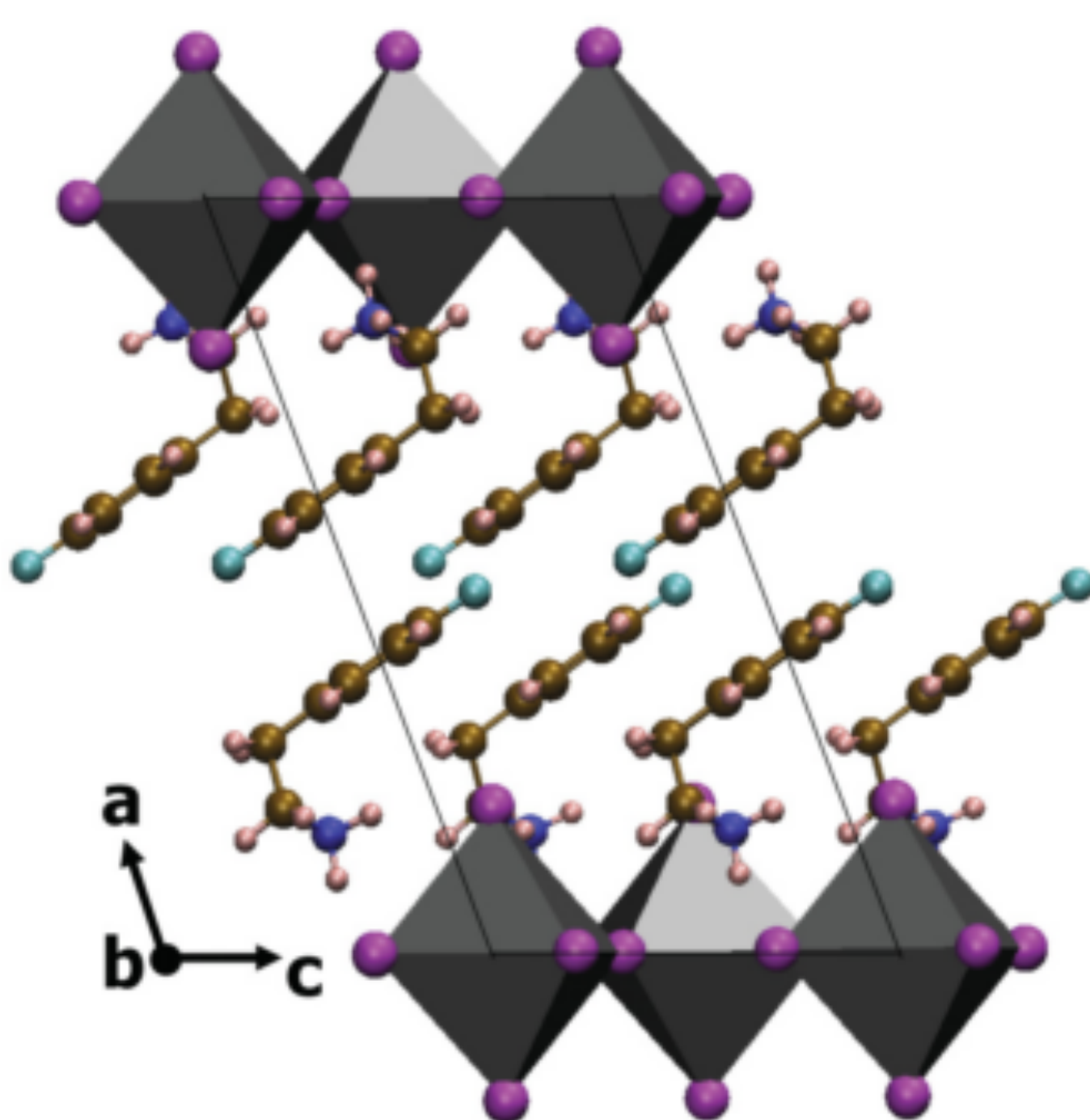
✧ Band gap at R

✧ selective SOC :

- larger with heavy B
- larger with heavy X
- consistent with atomic tables

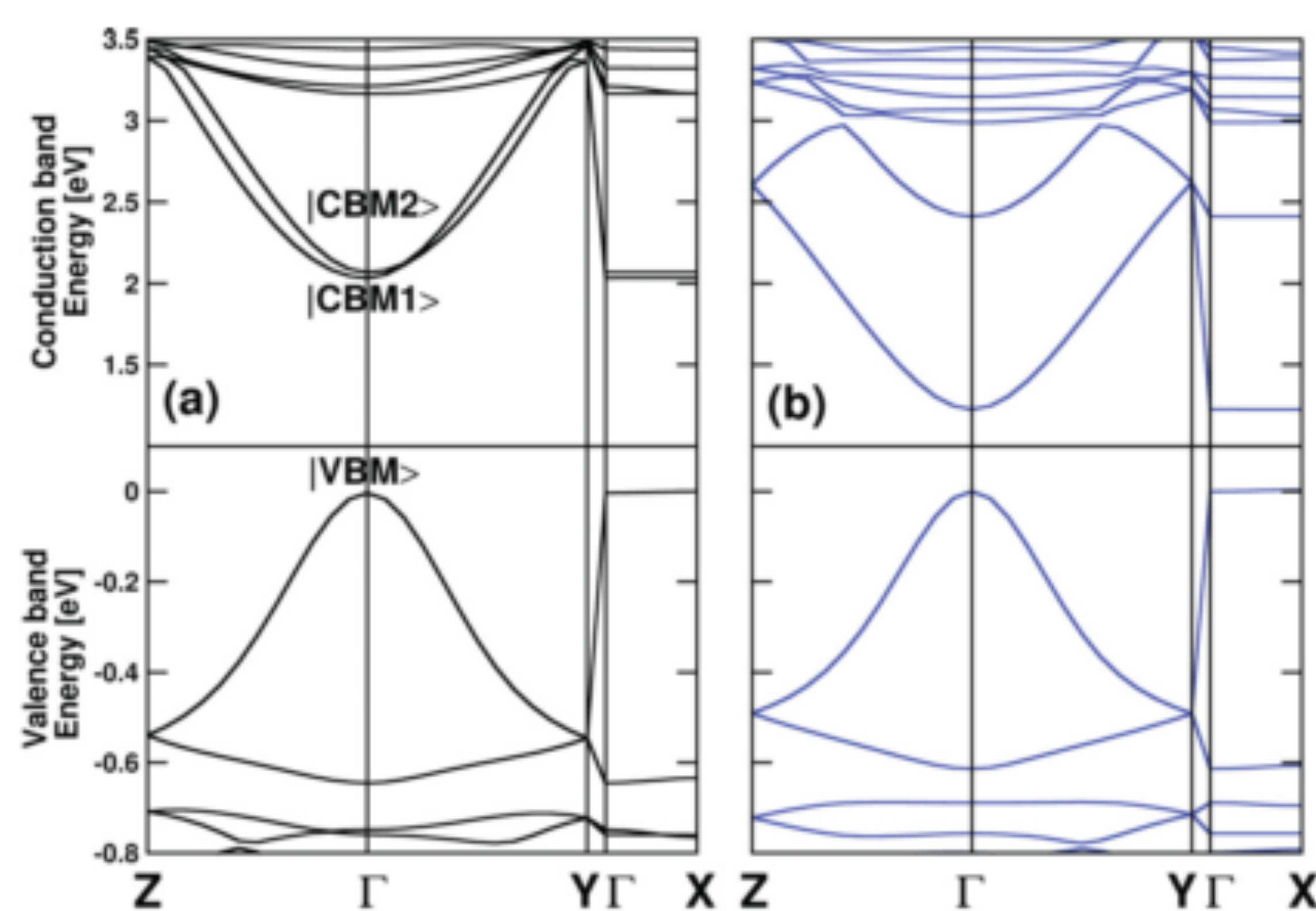
2D layered perovskites^[4]

Formula : A_2BX_4



2D structure:

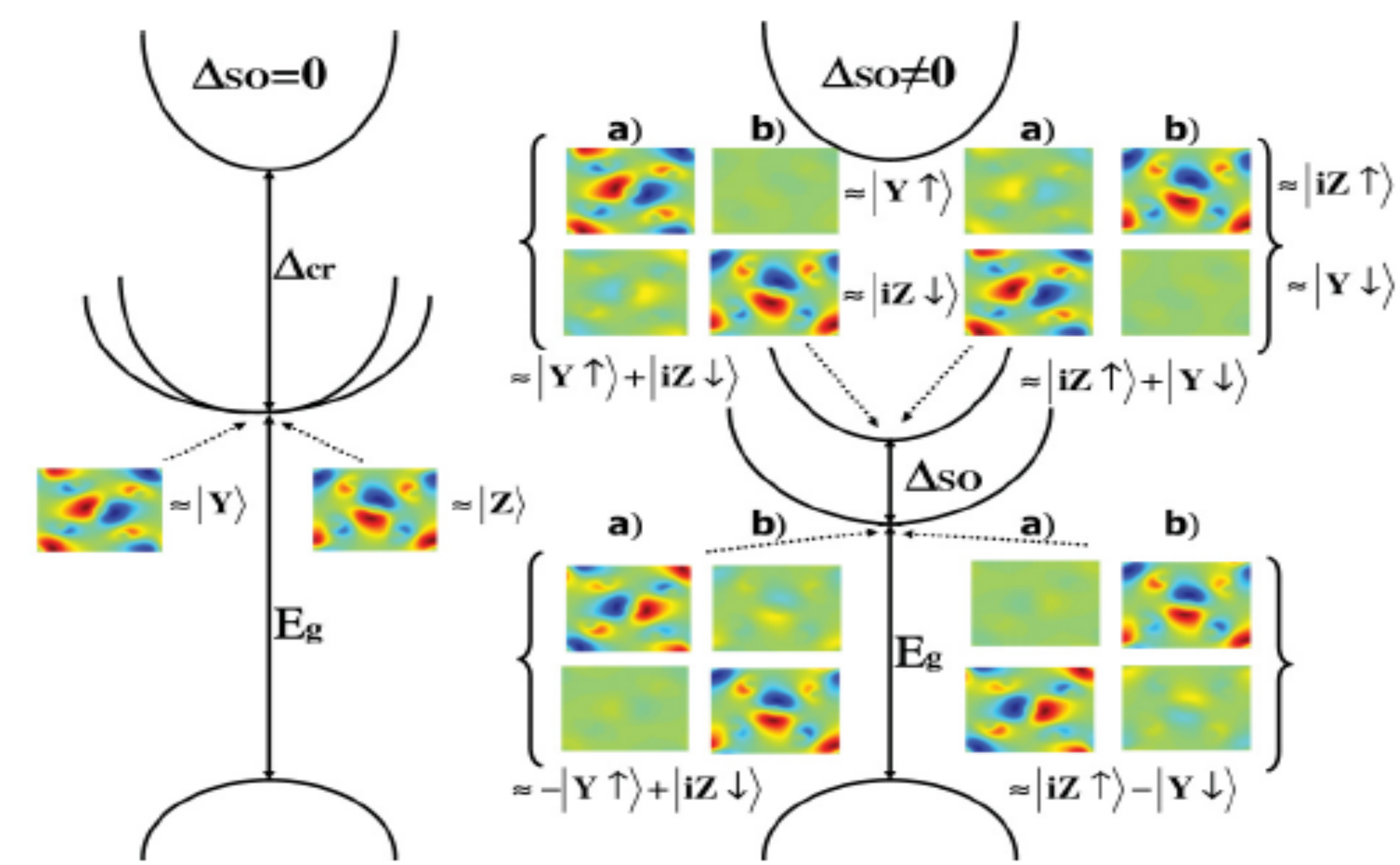
4F-PEPI
($[\text{pFC}_6\text{H}_5\text{C}_2\text{H}_4\text{NH}_3]_2\text{PbI}_4$)



✧ Band gap at Γ

✧ SOC effect important as in 3D

✧ Flat dispersion along Γ -X \rightarrow stacking axis



✧ Reverse band electronic states as compared to III-V conventional semiconductors

✧ Real ψ $|Y\rangle$ and $|Z\rangle$ without SOC are mixed by SOC into real and CBM components