Journal Name

ARTICLE TYPE

Cite this: DOI: 00.0000/xxxxxxxxxx

Supporting Information : Structure and Property Tunability in Monolayer Halide Lead-Free Double Hybrid Perovskites: Effects of Rashba and Biaxial Strain†

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Received Date
Accepted Date

DOI: 00.0000/xxxxxxxxxx

0.1 Electronic Structure

0.2 Optical Properties

0.3 About Experimental Device

Experimental device for 2D-materials strain usually available by bending it from various directions from other works[1].

Notes and references

1 H. J. Conley, B. Wang, J. I. Ziegler, J. Richard F. Haglund, S. T. Pantelides and K. I. Bolotin, *Nano Lett.*, 2013, **46**, 3626–3630.

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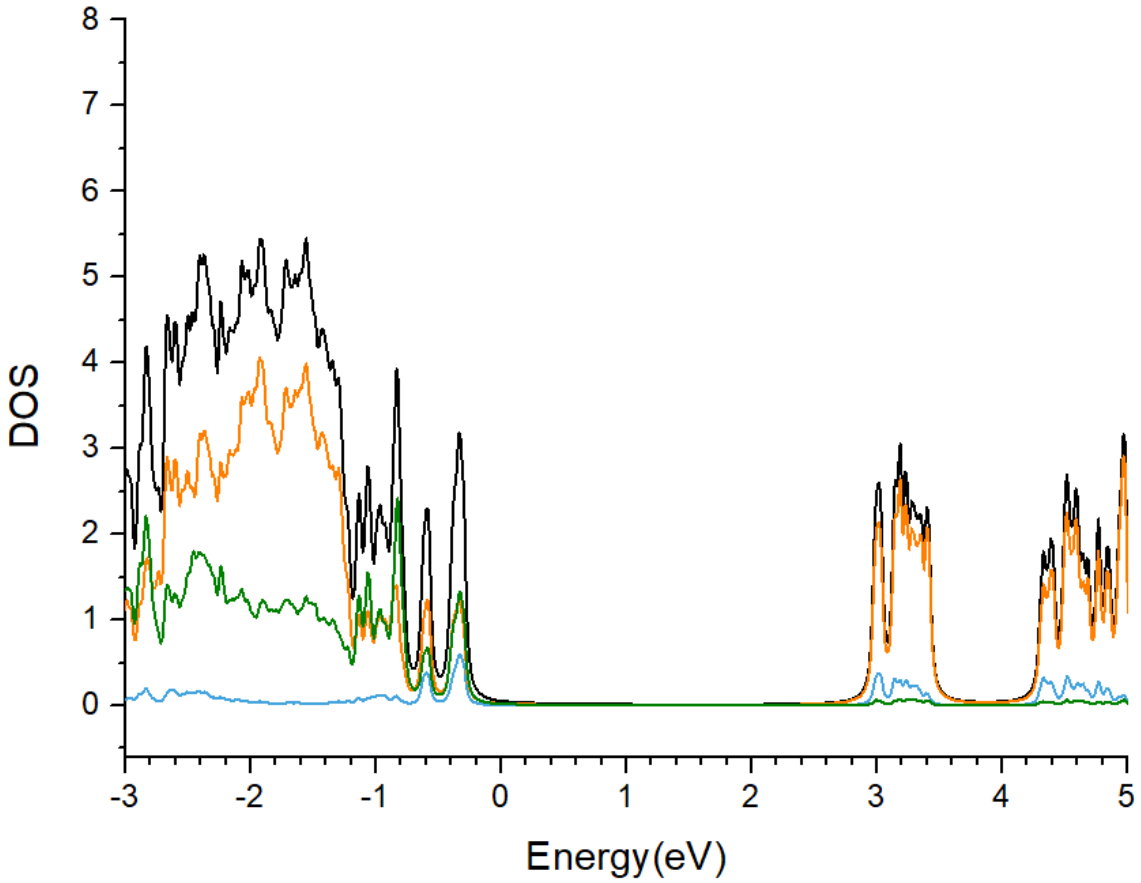

Fig. S 1 pDOS of bulk $MA_2[AgBi]Br_6$ calculated by PBE0+SOC.

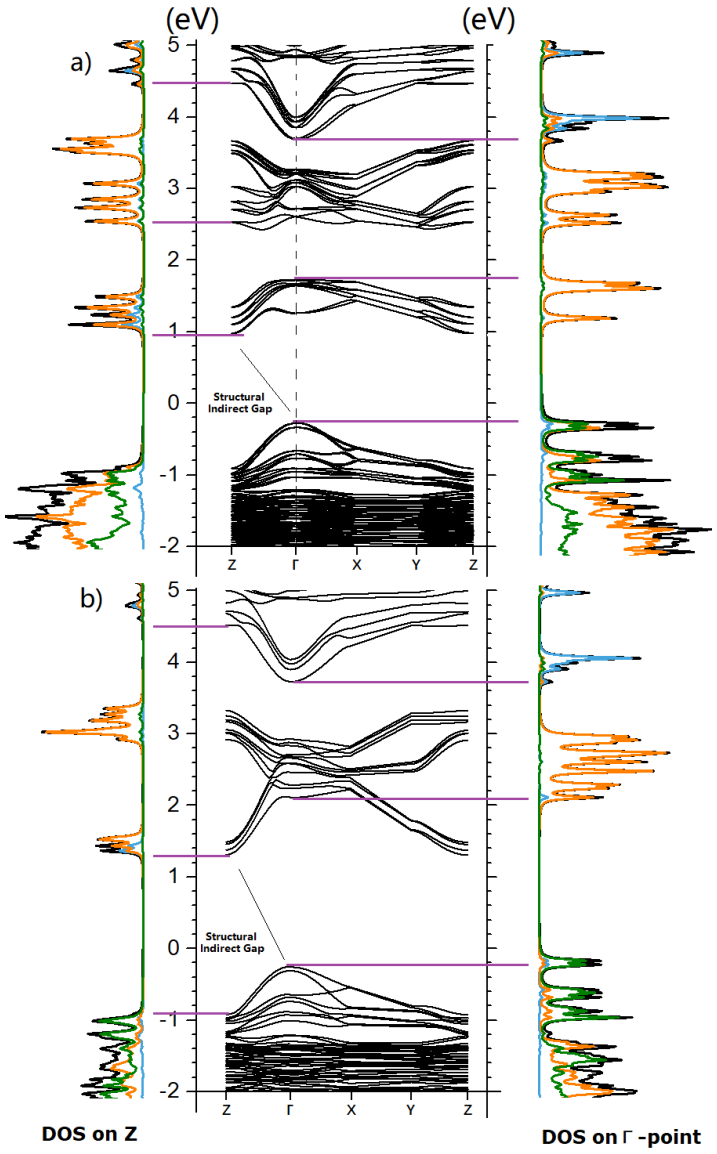

Fig. S 2 Calculated band structure and DOS of bulk $MA_2[AgBi]Br_6$ on Γ-point $(VBMpeak, rightpanel)$ and Γ-z point $(CBMvalley, leftpanel)$ by PBE , with (a) or without SOC (b).
Note that green DOSs represent for Ag-4d orbitals and orange ones represent for Br-4p and Bi-6p orbitals; light blue DOSs are s-orbitals contributed.

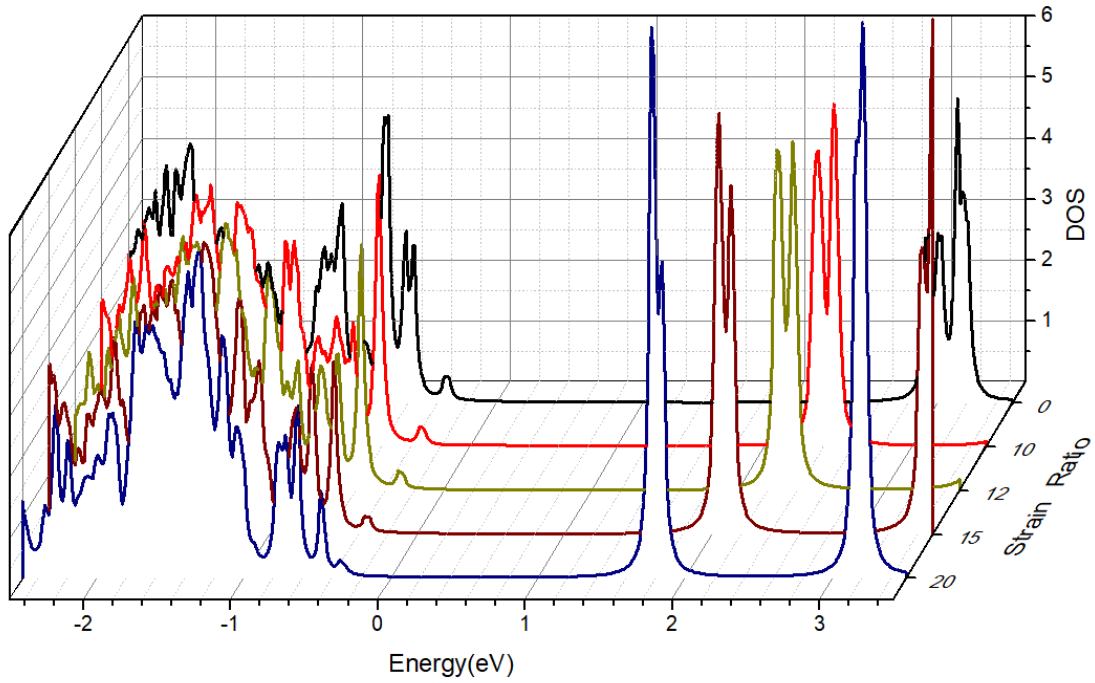

Fig. S 3 DOS of $MA_4[AgBi]Br_8$ stretched over 10%

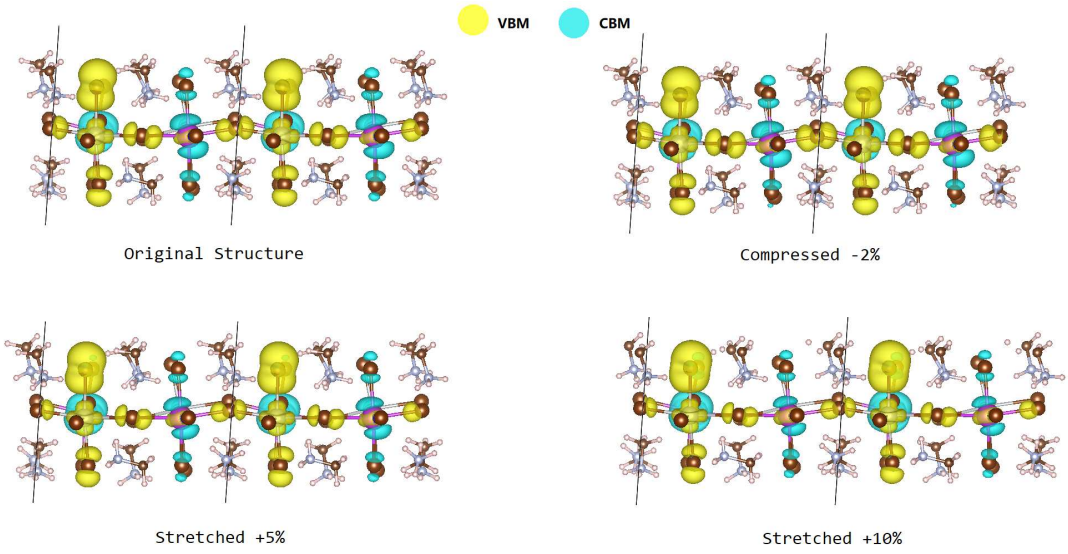

Fig. S 4 Charge distribution of Ag Bi and Br atoms in $MA_4[AgBi]Br_8$ strained differently
Notice that yellow for VBM and cyan for CBM.

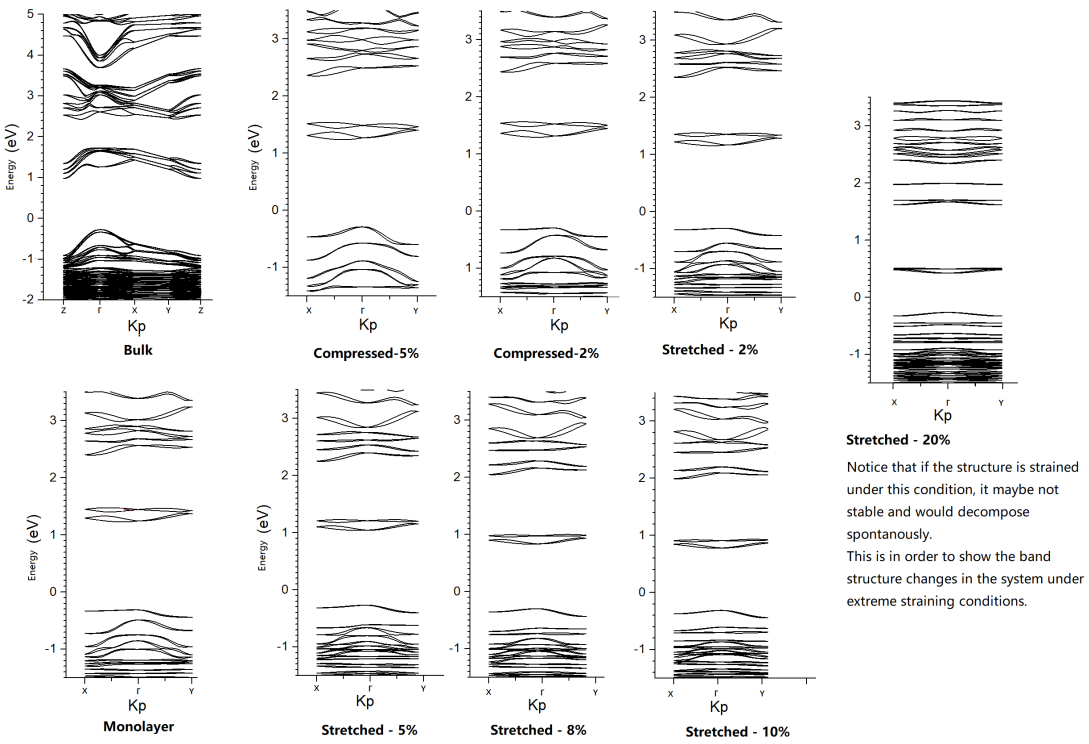

Fig. S 5 Band structure of $MA_4[AgBi]Br_8$ strained variously from -5% to 20% and bulk $MA_2[AgBi]Br_6$, by PBE+SOC.

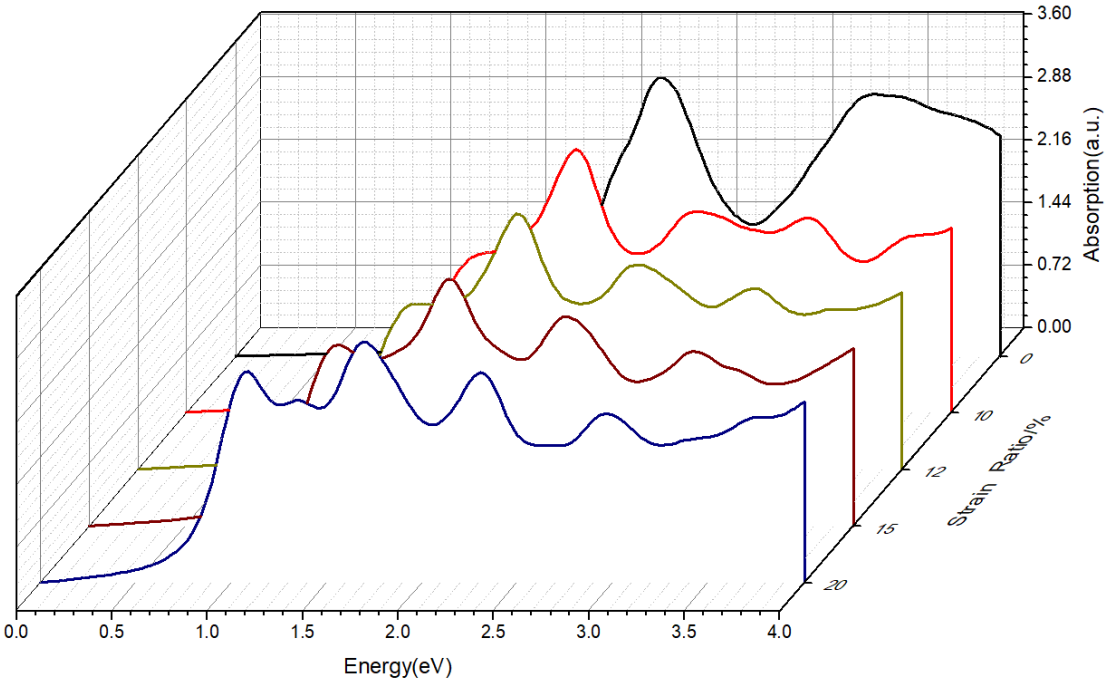

Fig. S 6 Absorption spectra of $MA_4[AgBi]Br_8$ with a strain over 10%

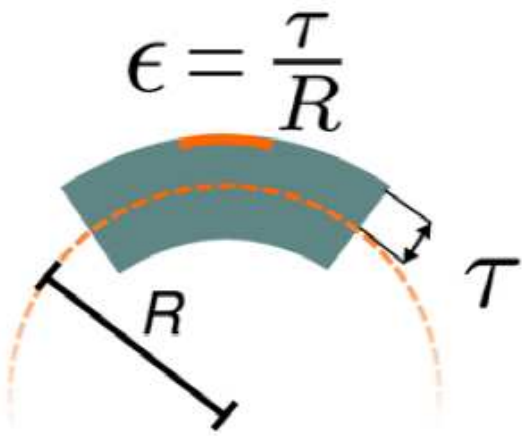

Fig. S 7 Experimental Device for Strain 2D Materials [1]

Schematic of the beam bending apparatus used to strain 2D materials
Notice that ε represents for strain ratio; τ for half of the thickness of the device and R for its curvature radius.