# Strain-induced half-valley metals and topological phase transitions in $MBr_2$ (M = Ru, Os) monolayers

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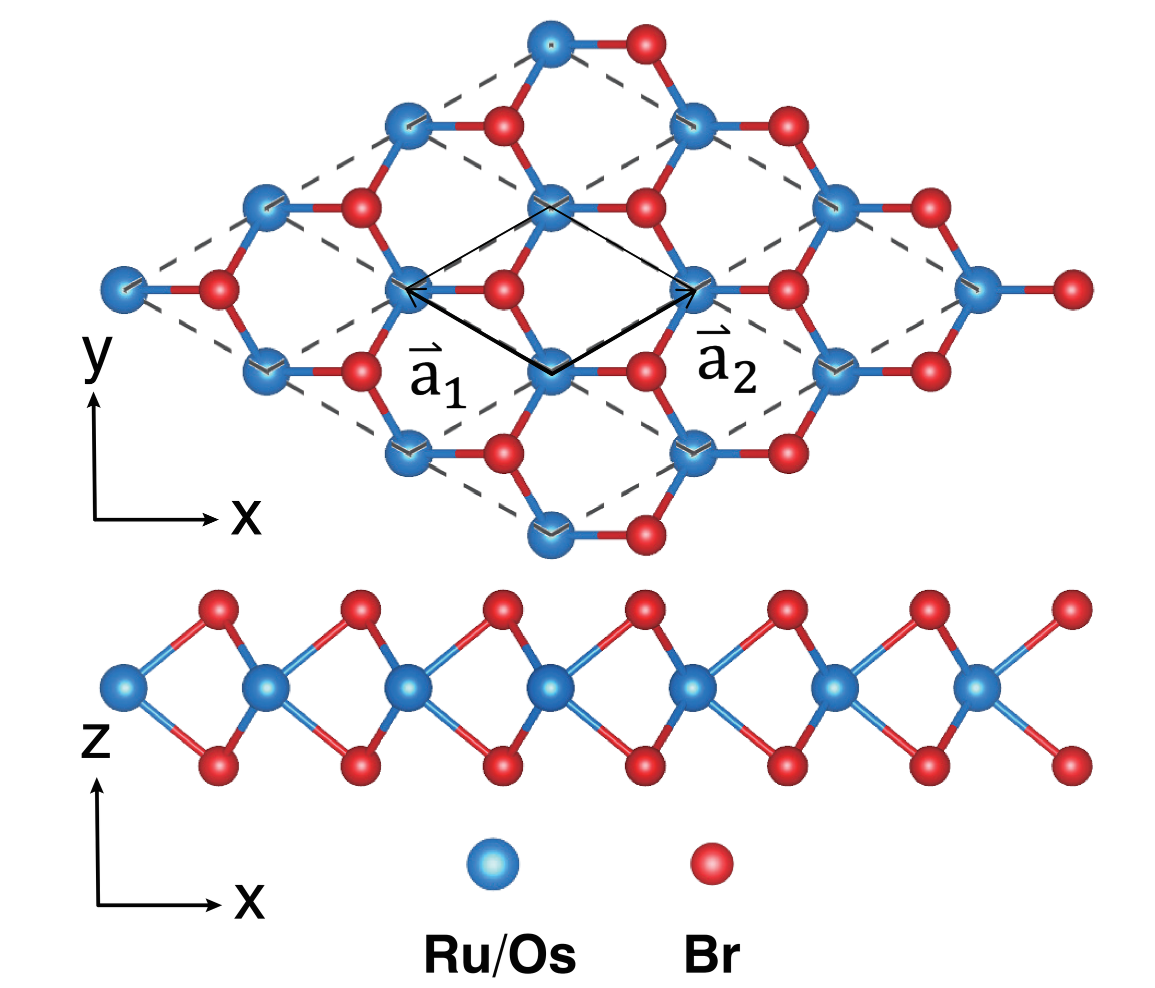
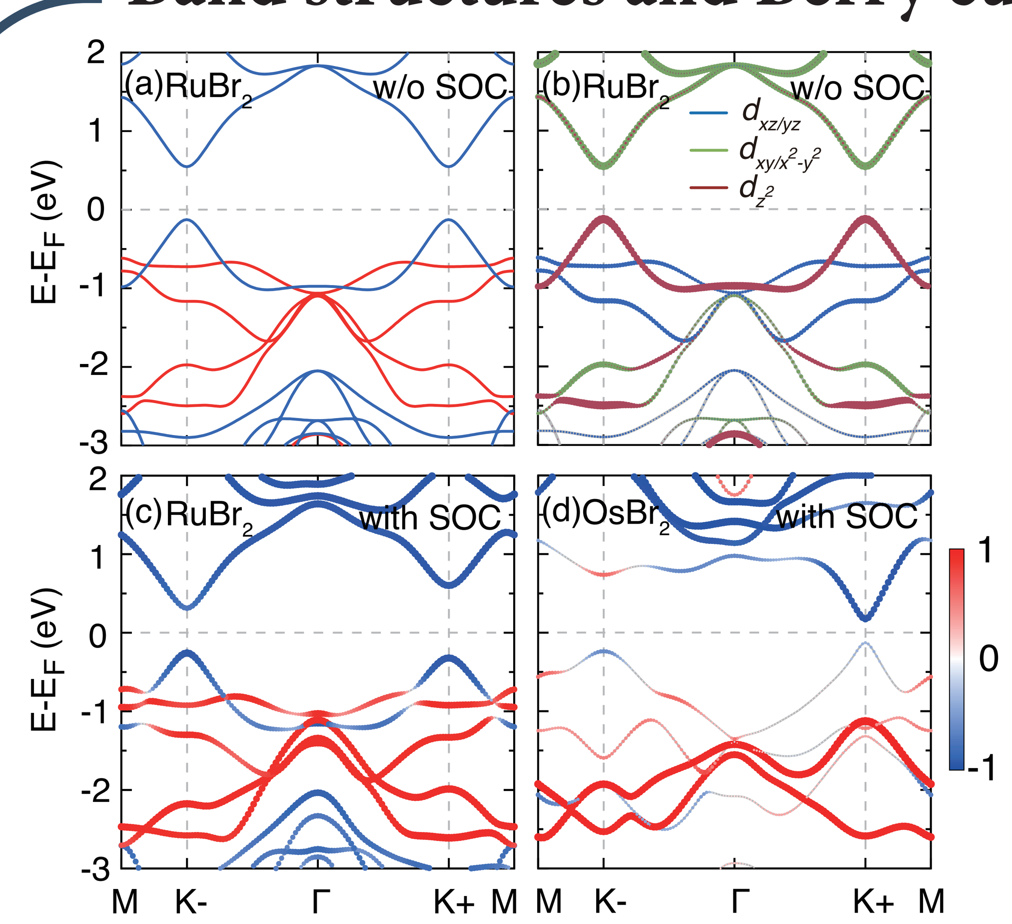
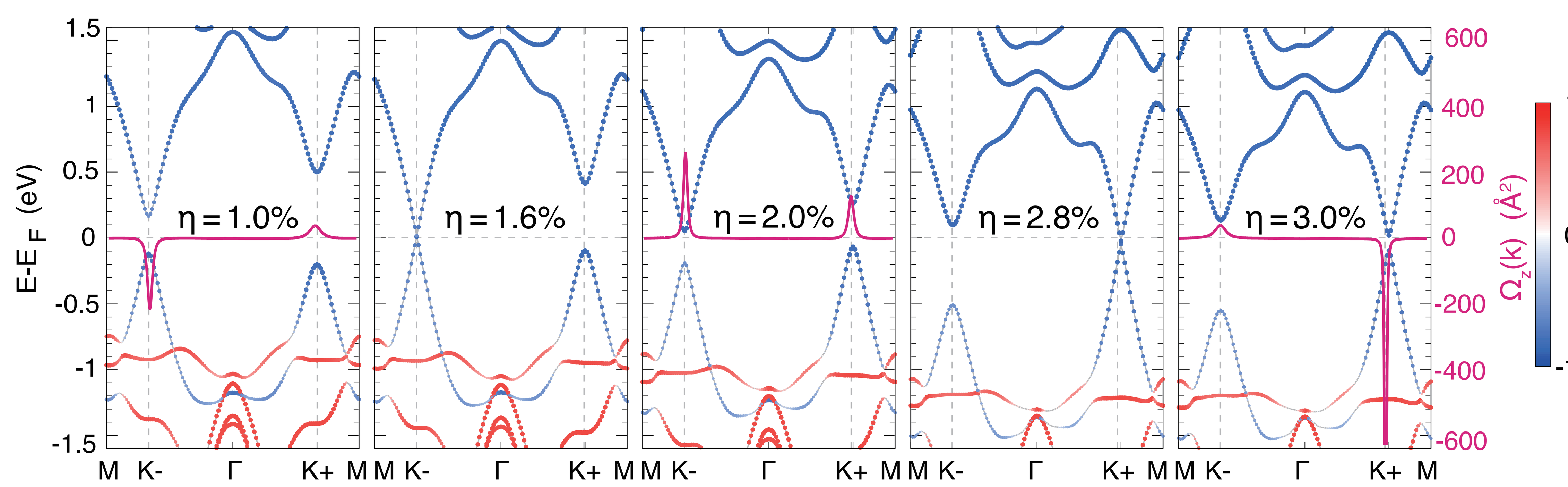
**Abstract:** The target of valleytronics developments is to manipulate the valley degree of freedom and utilize it in microelectronics as charge and spin degrees of freedom. Based on first-principles calculations, we demonstrate that $MBr_2$ (M = Ru, Os) monolayers are intrinsically ferrovalley materials with large valley polarization up to 530 meV, a record value. Compressive strain can induce phase transitions in the materials from ferrovalley insulators to complete valley polarized metals, called half-valley metals, in analogy to the concept of half-metals in spintronics. With the increase of the strain, the materials become Chern insulators, whose edge states are chiral-spin-valley locking.The phase transition is caused by sequent band inversions of the $d_{xy}/d_{x^2-y^2}$ and $d_{z^2}$ orbitals at K- and K+ valleys, analyzed based on a strained $\boldsymbol{k} \cdot \boldsymbol{p}$ model. Our work provides a pathway for carrying out low dissipation electronics devices with complete spin and valley polarizations.

## Structures




## Band structures and Berry curvatures



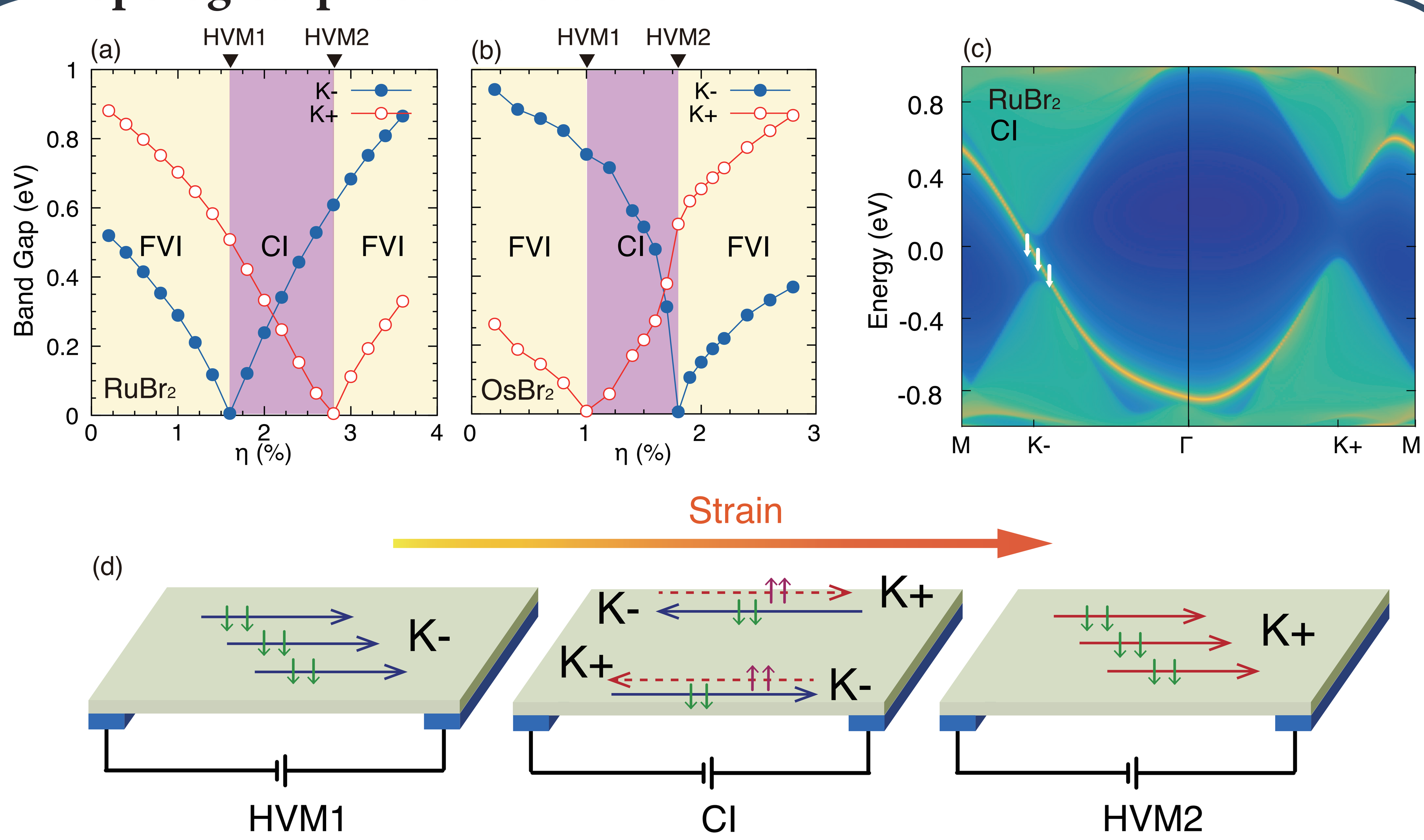




Band structures of the $RuBr_2$ monolayer with SOC under compressive strain with different magnitudes. The red and blue colors indicate the spin-up and spin-down bands, respectively. The magenta curves denote the Berry curvatures of the corresponding system.

## The two-band strained $k{\cdot}p$ model

$$H(\mathbf{k}) = \left(f_0 - sM - 2f_3\varepsilon + \frac{1}{2}s\tau\lambda_c\right)\sigma_0 + \left(\frac{1}{2}s\tau\lambda_c - \frac{1}{2}f_1 + 2f_4\varepsilon\right)\sigma_z + f_2 a\tau k_x\sigma_x - f_2 a k_y\sigma_y$$

## Topological phase transitions

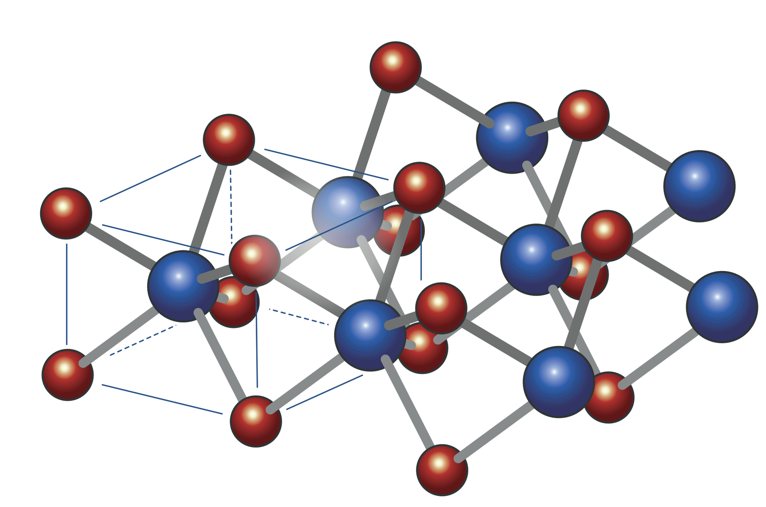



(a)/(b) The phase diagram of the $RuBr_2/OsBr_2$ monolayer as a function of compressive strain. HVM: half-valley metal; FVI: ferrovalley insulator; CI: Chern insulator.

(c) The 100% spin-polarized chiral edge state is locked with the valley index and spin direction.

(d) Schematic diagrams of the electronic device rudiments made of the $RuBr_2$ monolayer tuned by the compressive strain.

**Conclusions:** **(a)** $RuBr_2$ and $OsBr_2$ monolayers are intrinsically ferrovalley materials with large spontaneous valley polarization. **(b)** Half-valley metallic states, with 100% valley polarization, are obtained for $RuBr_2$ under compressive strain. **(c)** Between the two half-valley metallic states, both of the materials become Chern insulators with exotic chiral-spin-valley locking edge states.



## References

D. Xiao, W. Yao, and Q. Niu, *Phys. Rev. Lett.* 99, 236809 (2007)

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