Two-dimensional ferromagnetic semiconductor VBr_3 with tunable anisotropy

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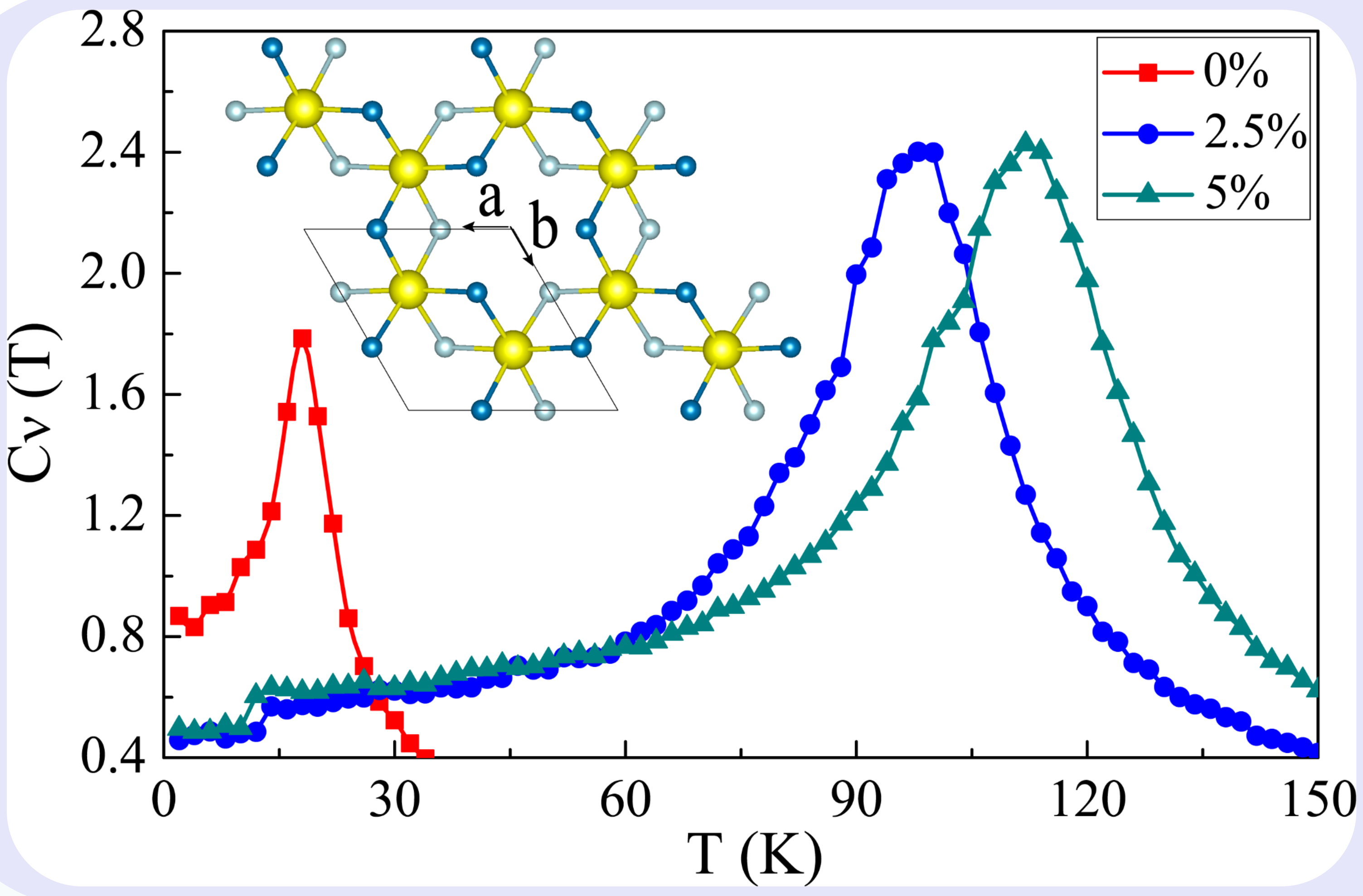
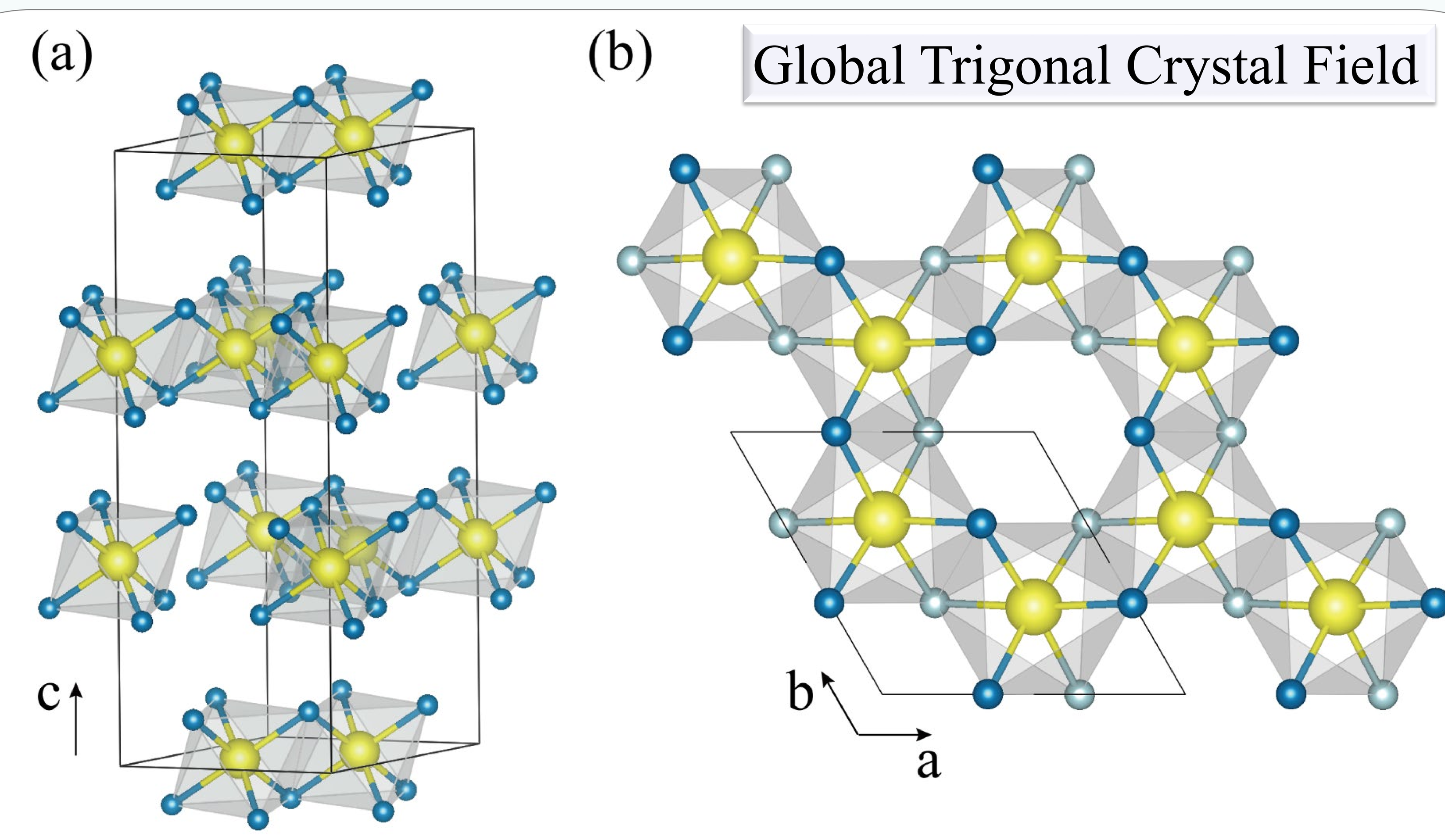
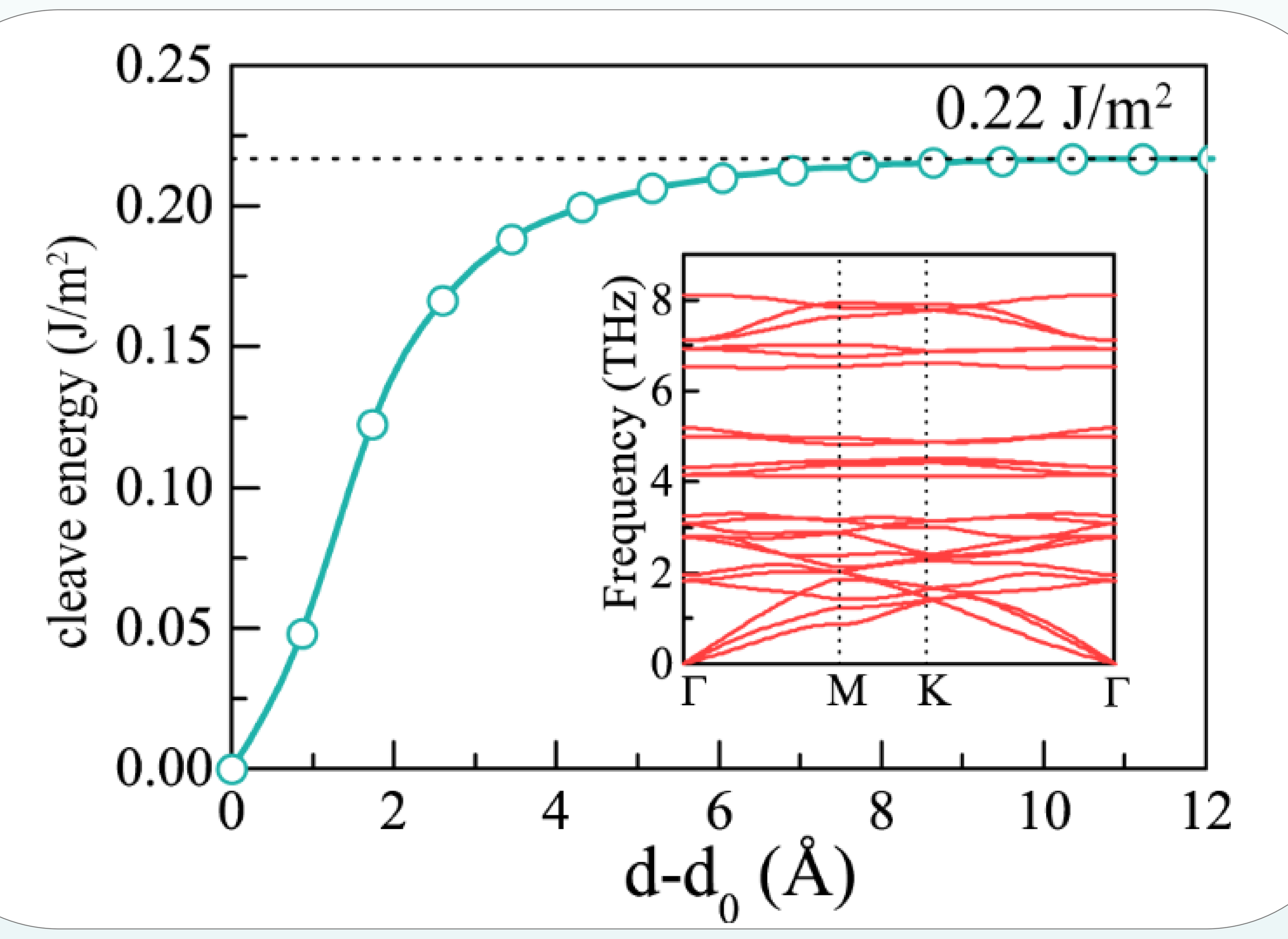
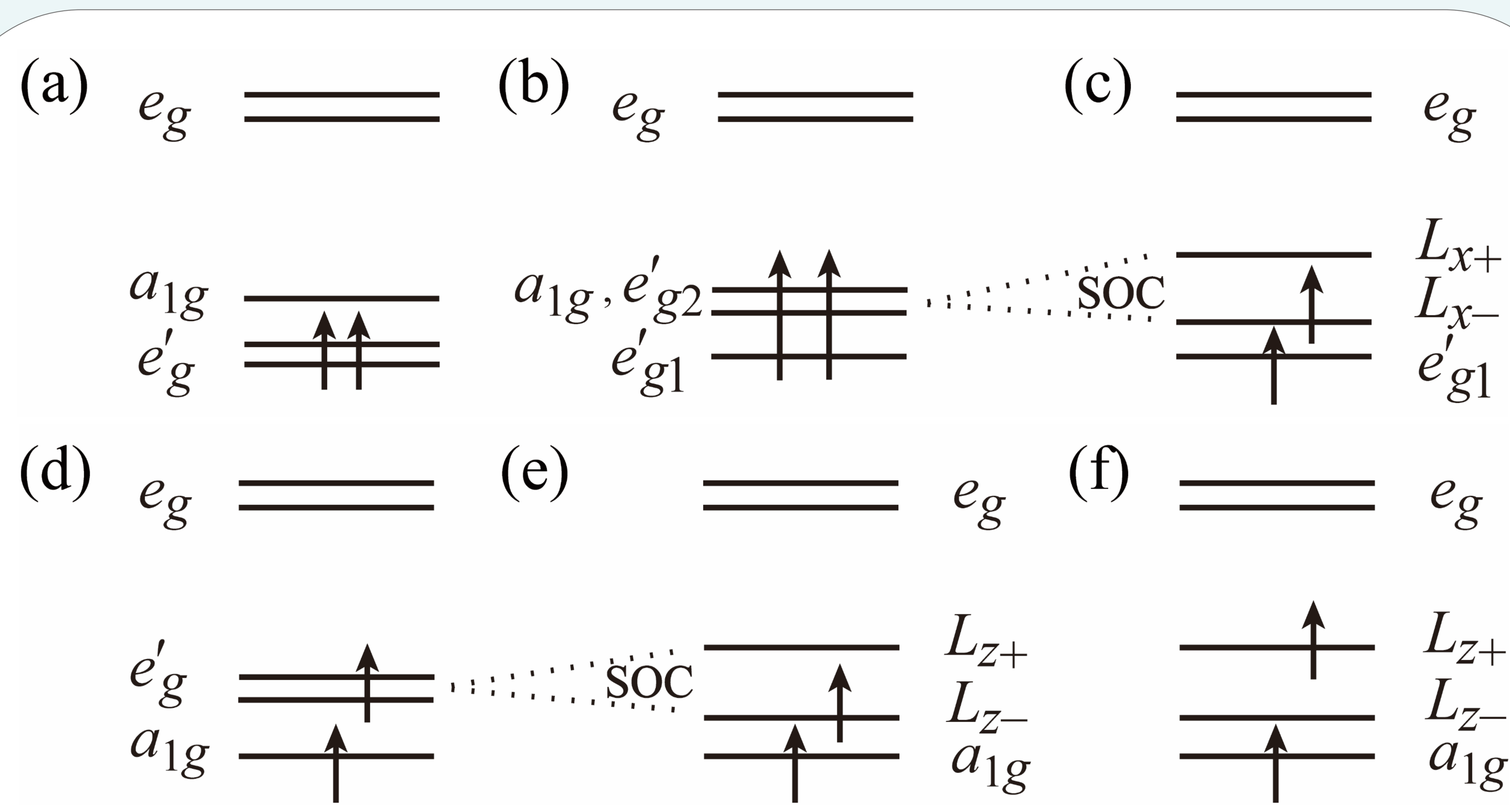
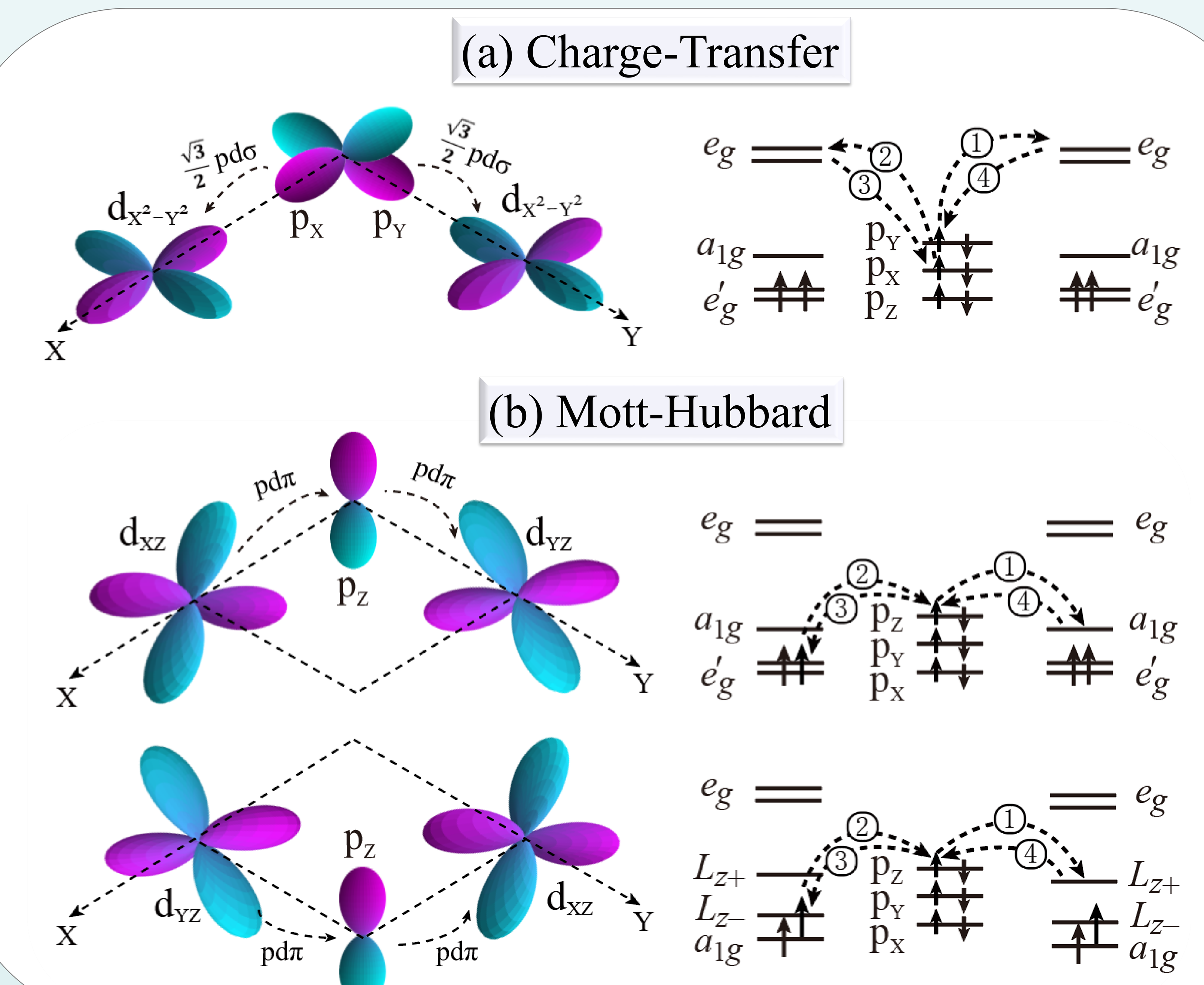


Two-dimensional ferromagnets have attracted widespread attention due to their prospects in spintronic applications. Here we explore the electronic structure and magnetic properties of VBr_3. VBr_3 bulk and monolayer have the $e_g'^2$ (M_{orb}= −0.23 μ_B) ground state and possess a **weak in-plane** anisotropy. More interestingly, a **tensile strain** on the semiconducting VBr_3 monolayer tunes the ground state into $a_{1g}^1 L_{z-}^1$ (M_{orb}= −1.15 μ_B) and thus produces a **strong out-of-plane** anisotropy. Then, the significantly enhanced FM superexchange and single ion anisotropy would raise T_C from 20 K for the bare VBr_3 monolayer to 100-115 K under a 2.5%-5% strain. Therefore, VBr_3 would be a promising 2D FM semiconductor with a tunable anisotropy.









Strain	States	ΔE (meV/fu)	M_{spin} (μ_B)	M_{orb} (μ_B)
0%	$e_g'^2$, //	0.0	1.87	−0.23
	$e_g'^2$, // (AF)	7.9	1.84	−0.21
	$e_g'^2$, ⊥	2.0	1.86	0.00
	$a_{1g}^1 L_{z-}^1$, ⊥	12.0	1.91	−1.15
2.5%	$a_{1g}^1 L_{z-}^1$, ⊥	0.0	1.92	−1.16
	$e_g'^2$, //	80.9	1.87	−0.44
5%	$a_{1g}^1 L_{z-}^1$, ⊥	0.0	1.92	−1.17
	$e_g'^2$, //	141.6	1.87	−0.41

$$H = -D\sum_i (S_i^z)^2 - \frac{J}{2}\sum_{\langle ij\rangle} \vec{S_i}\cdot\vec{S_j} - \frac{J'}{2}\sum_{\langle ij\rangle} S_i^z \cdot S_j^z$$

Strain	D (meV)	J (meV)	J' (meV)	T_C (K)
0%, //	−1.9	2.6	−0.06	20
2.5%, ⊥	15.2	10.8	−0.15	100
5%, ⊥	13.9	12.8	−0.02	115

VBr_3 monolayer: an appealing 2D semiconductor with a strong strain tunability of its ferromagnetic order and anisotropy