

**Tuning the spin-orbit coupling, magnetic proximity and band hybridization in
Fe(001)/MgO(n MLs)/MoS₂ multilayers
SUPPLEMENTARY MATERIALS**

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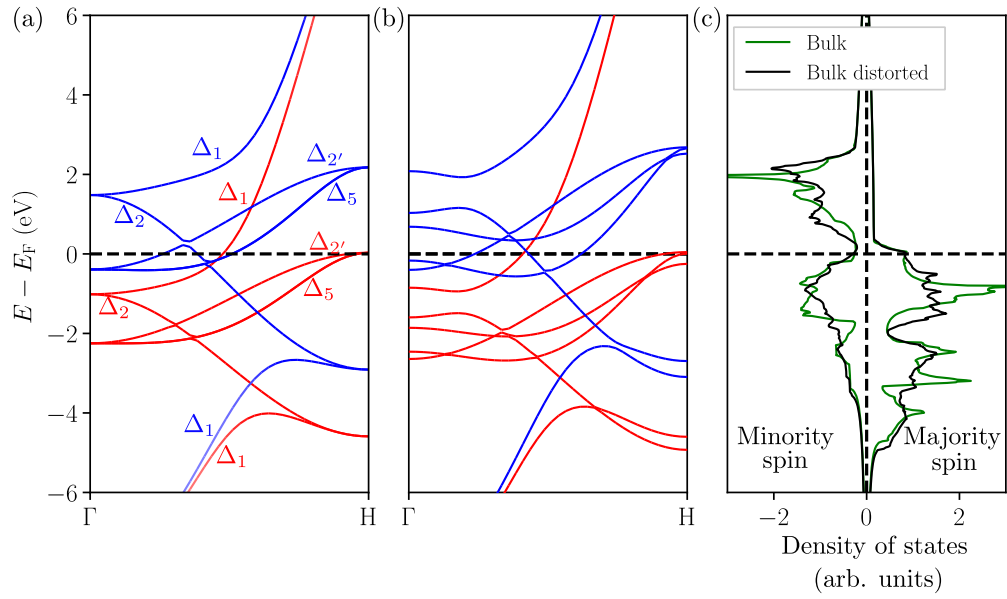


Figure S 1. (a) Band structure of the cubic Fe crystal for wave vectors in the [001] direction; majority and minority bands are respectively shown with red and blue lines. (b) Same as in (a), but for the distorted Fe crystal. (c) comparison of the density of state (DOS) curves calculated for the cubic and the distorted Fe crystals.

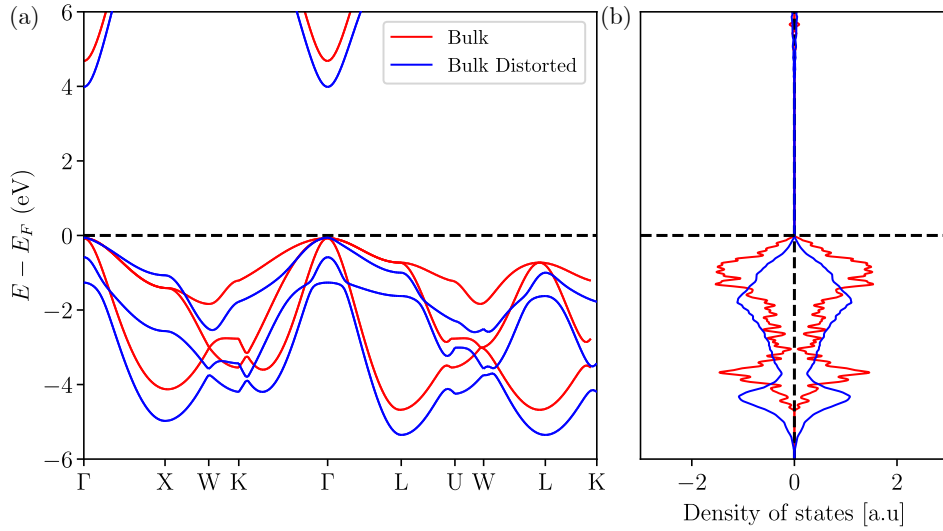


Figure S 2. (a) Band structure of the cubic (red lines) and distorted (blue lines) MgO crystals. (c) Comparison of the density of state (DOS) curves calculated for the cubic (red lines) and distorted (blue lines) MgO crystals.

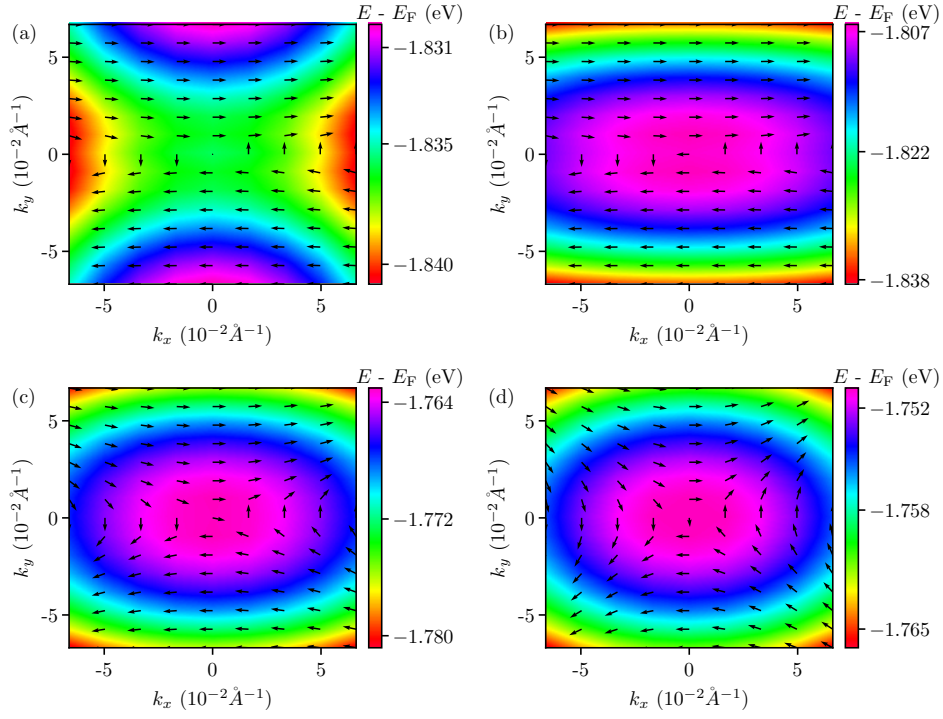


Figure S 3. Modulus and direction of the in-plane projection of the spin vector calculated near Γ from first principles, for the highest energy valence band of MoS₂ in V/MgO/MoS₂ multilayers with $t_{\text{MgO}} = 4$ MLs (a), 5 MLs (b), 6 MLs (c) and 7 MLs (d). The color code shows the dispersion of the valence band near Γ .

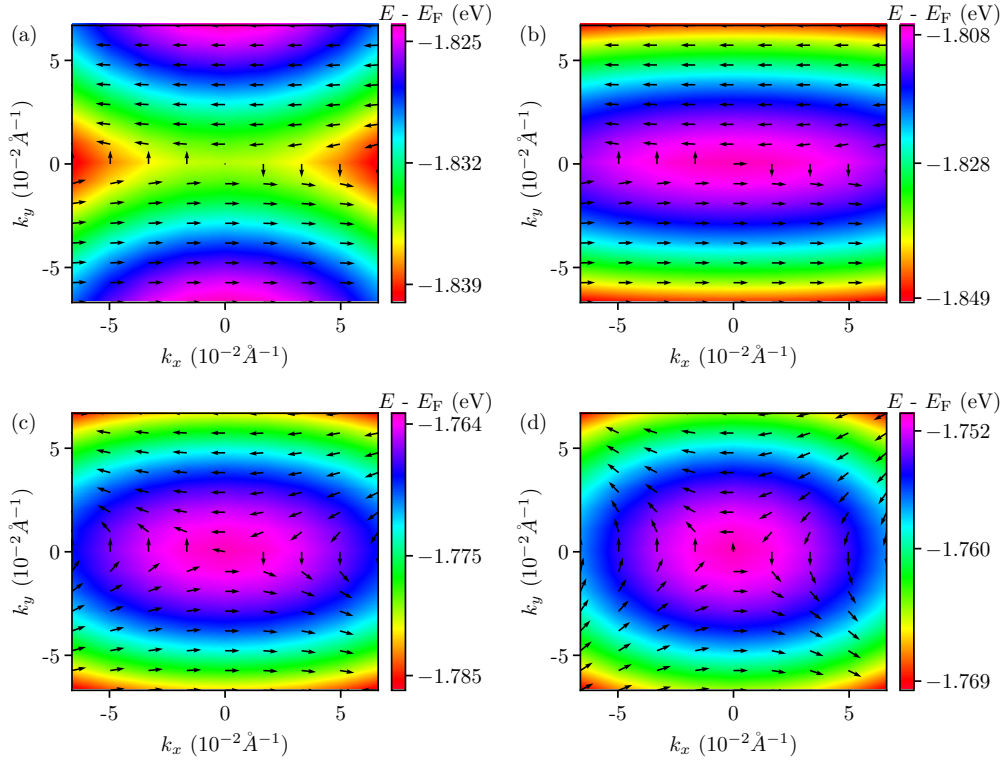


Figure S 4. Same as Fig. S 3, but for the second highest energy valence band at Γ of MoS₂ in V/MgO/MoS₂ multilayers.

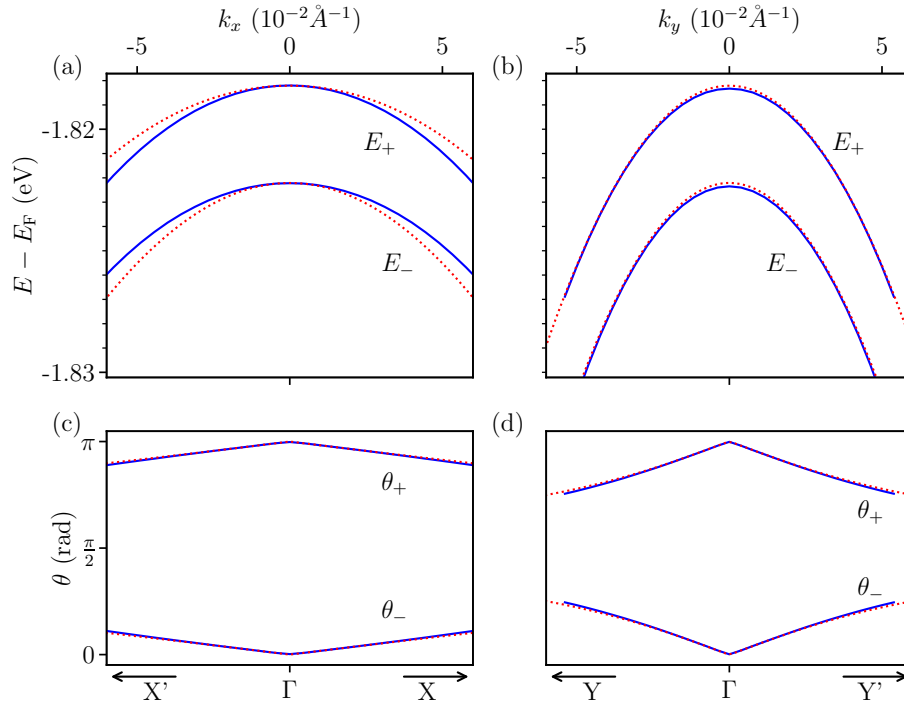


Figure S 5. (a) Dispersion of the MoS₂ valence bands of the multilayer Fe/MgO(4MLs)/MoS₂, for Bloch vectors along Γ -X; the blue solid lines correspond to the first-principles data, while the red dotted lines correspond to the eigenvalues E_+ and E_- of the effective Hamiltonian. (b) Same as (a), but for Bloch vectors along Γ -Y. (c) Angle θ between the spin vector and the z axis, calculated for the multilayer Fe/MgO(4MLs)/MoS₂ and for Bloch vectors along Γ -X; the blue solid lines correspond to the first-principles data and the red dotted lines to the angles θ_+ and θ_- calculated from the eigenvectors of the effective Hamiltonian. (d) Same as (c), but for Bloch vectors along Γ -Y.

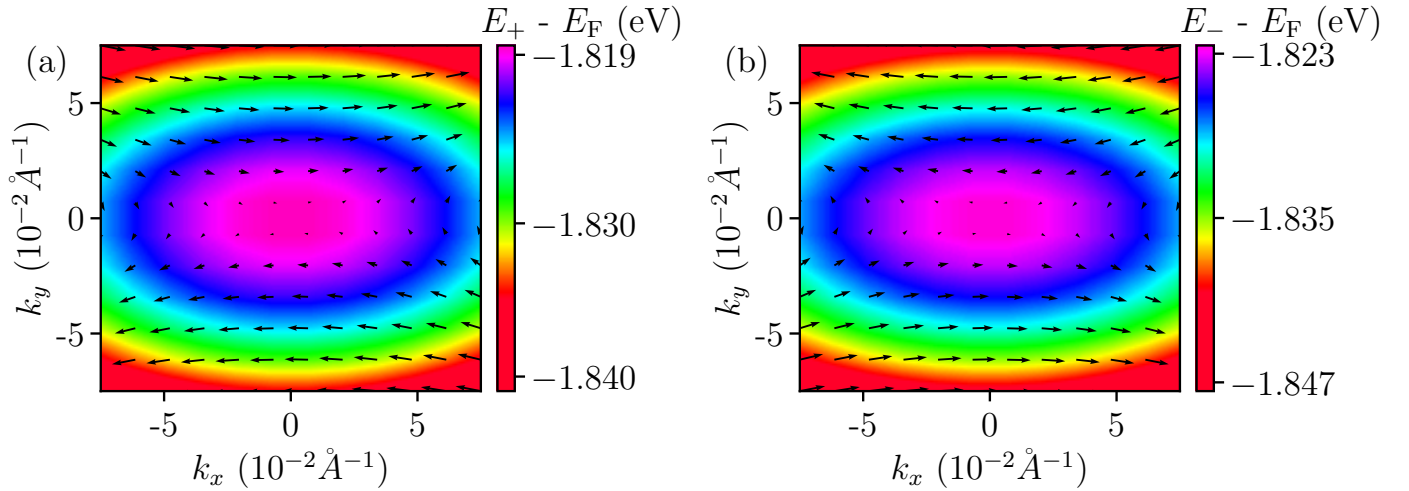


Figure S 6. Modulus and direction of the in-plane projection of the spin vector, calculated for the multilayer Fe/MgO(4MLs)/MoS₂ (a) using the angle ϕ_+ and (b) using the angle ϕ_- .

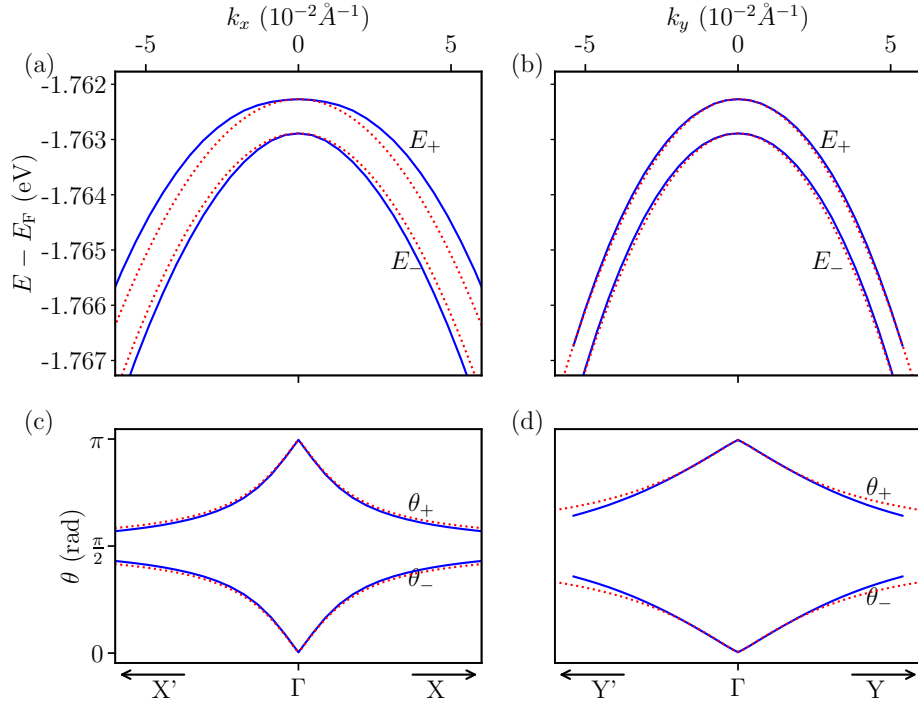


Figure S 7. Same as in Fig. S 5, but for the multilayer Fe/MgO(6MLs)/MoS₂.

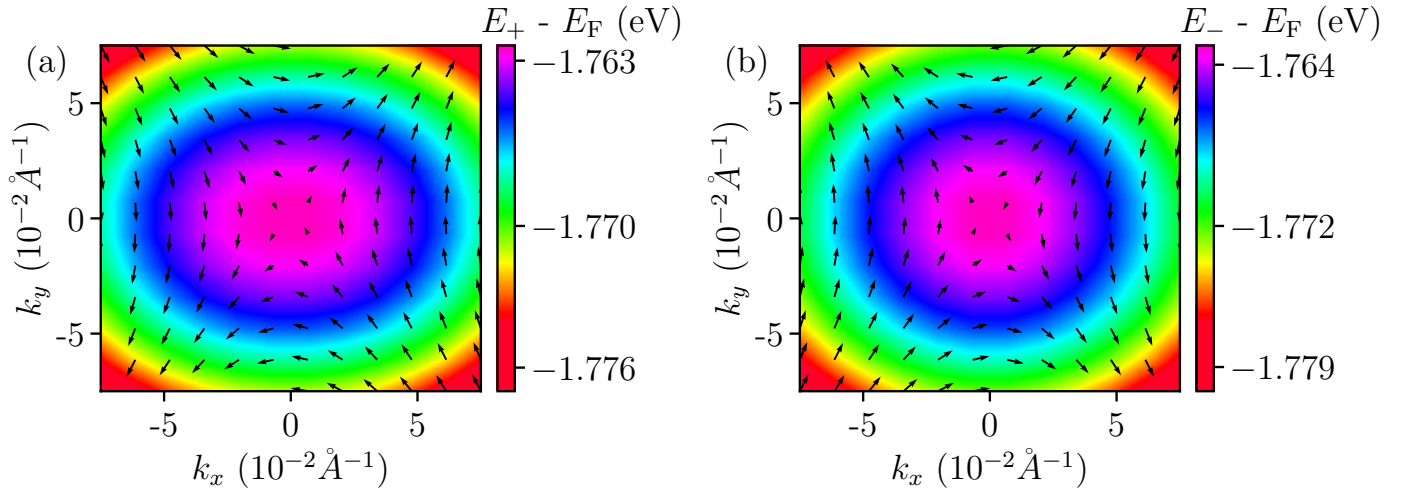


Figure S 8. Same as in Fig. S 6, but for the multilayer Fe/MgO(6MLs)/MoS₂.

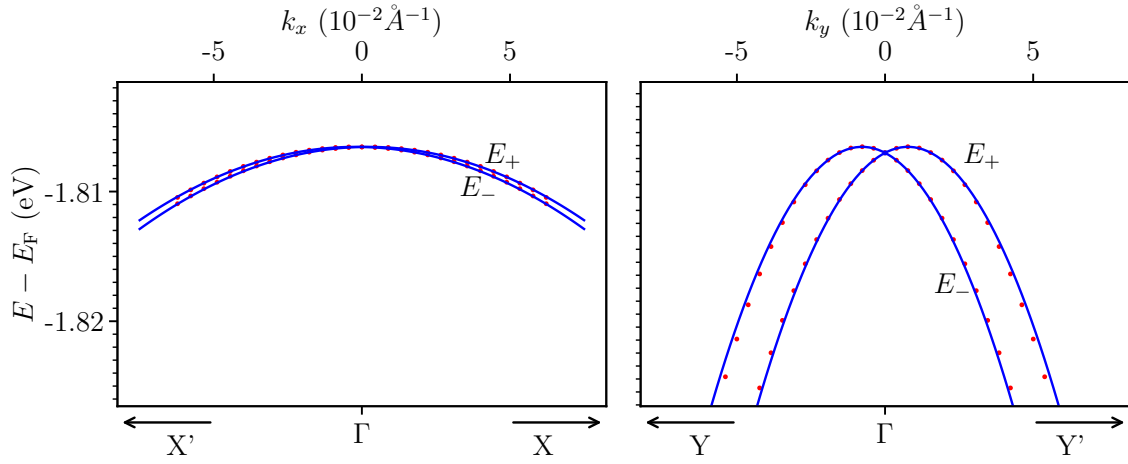


Figure S 9. Dispersion of the MoS₂ valence bands of the multilayer V/MgO(5MLs)/MoS₂, for Bloch vectors along Γ -X (left panel) and Γ -Y (right panel); the blue solid lines correspond to the first-principles data, while the red dotted lines correspond to the eigenvalues E_+ and E_- of the effective Hamiltonian.

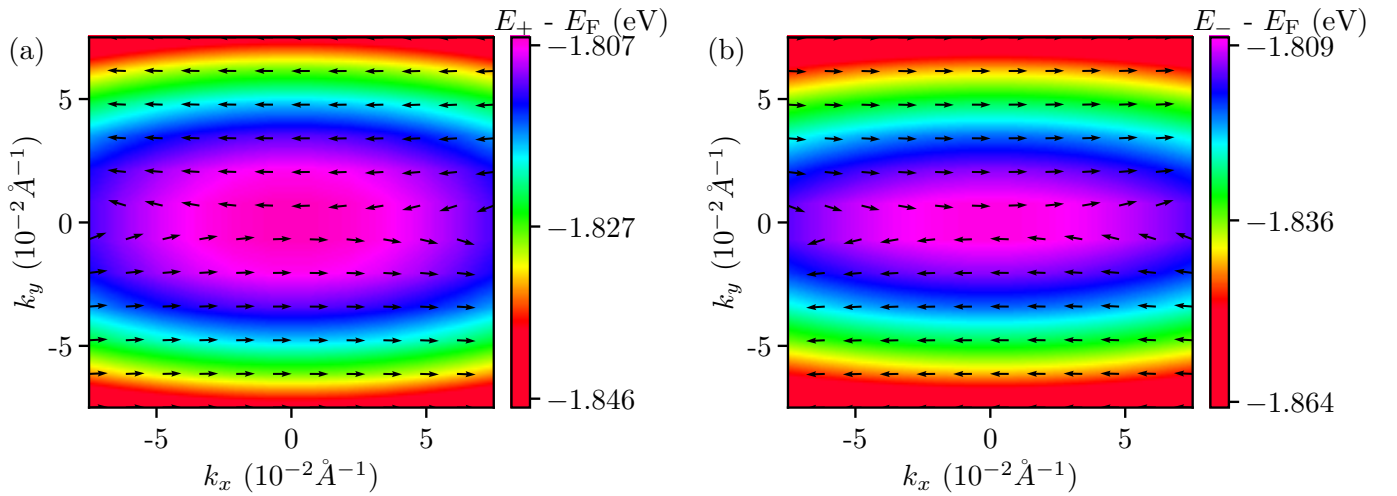


Figure S 10. Direction of the spin vector, calculated for the multilayer V/MgO(5MLs)/MoS₂ using the angle ϕ_+ (left panel) and the angle ϕ_- (right panel).

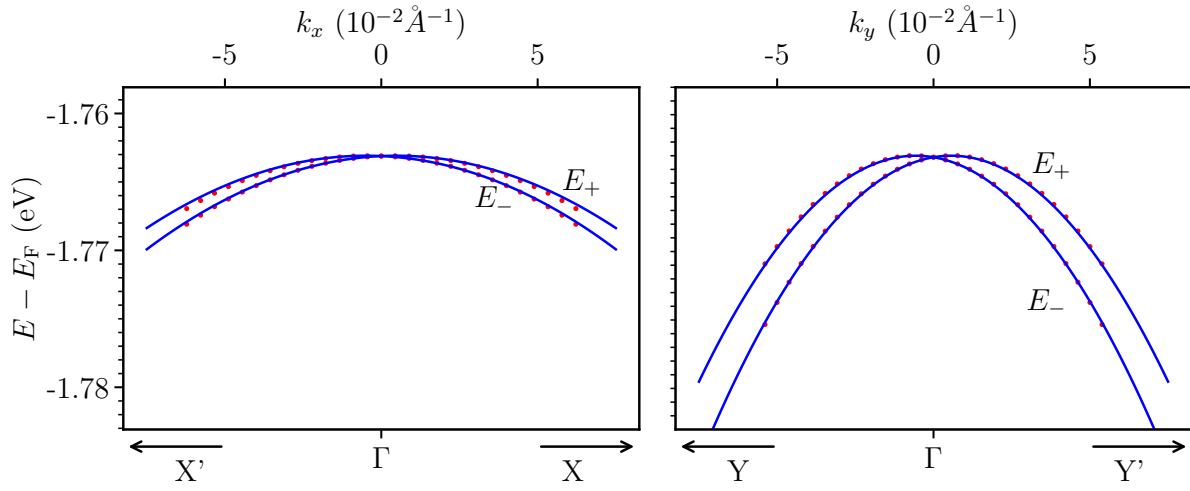


Figure S 11. Same as in Fig. S 9, but for the multilayer V/MgO(6MLs)/MoS₂.

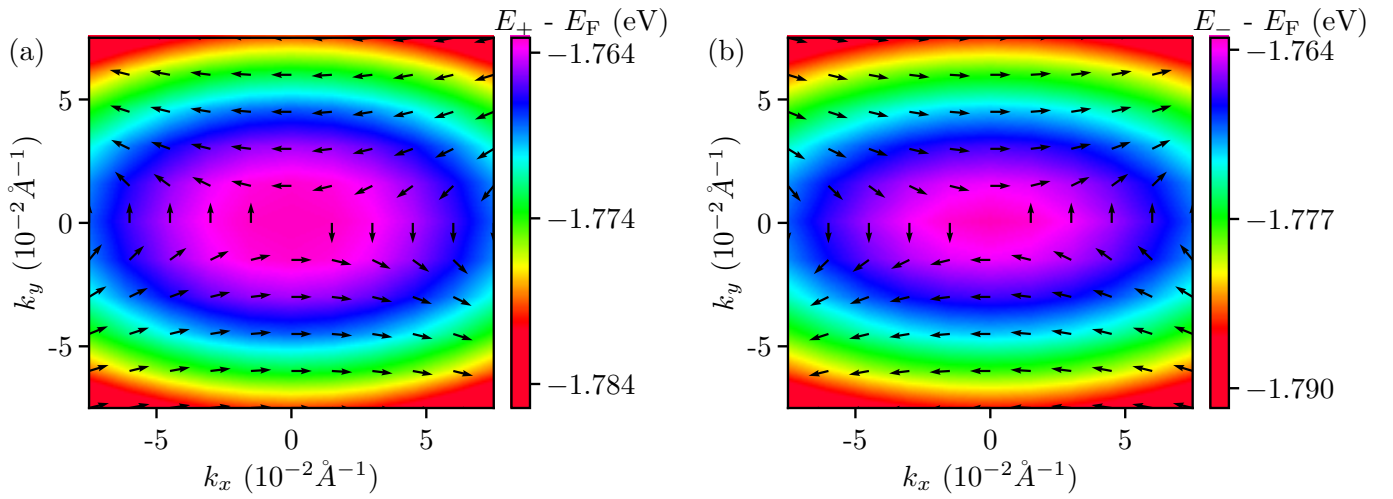


Figure S 12. Same as in Fig. S 10, but for the multilayer V/MgO(6MLs)/MoS₂.

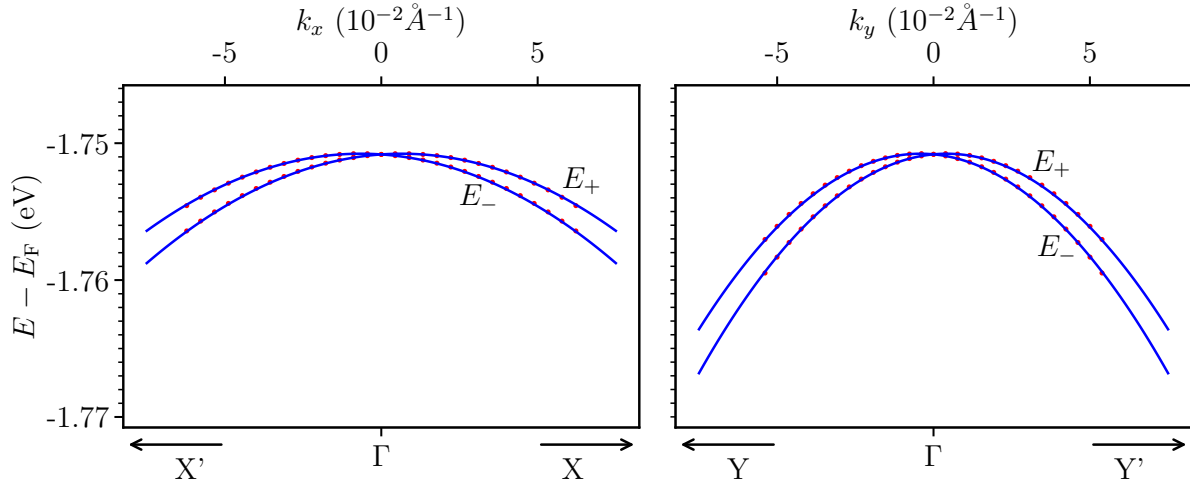


Figure S 13. Same as in Fig. S 9, but for the multilayer V/MgO(7MLs)/MoS₂.

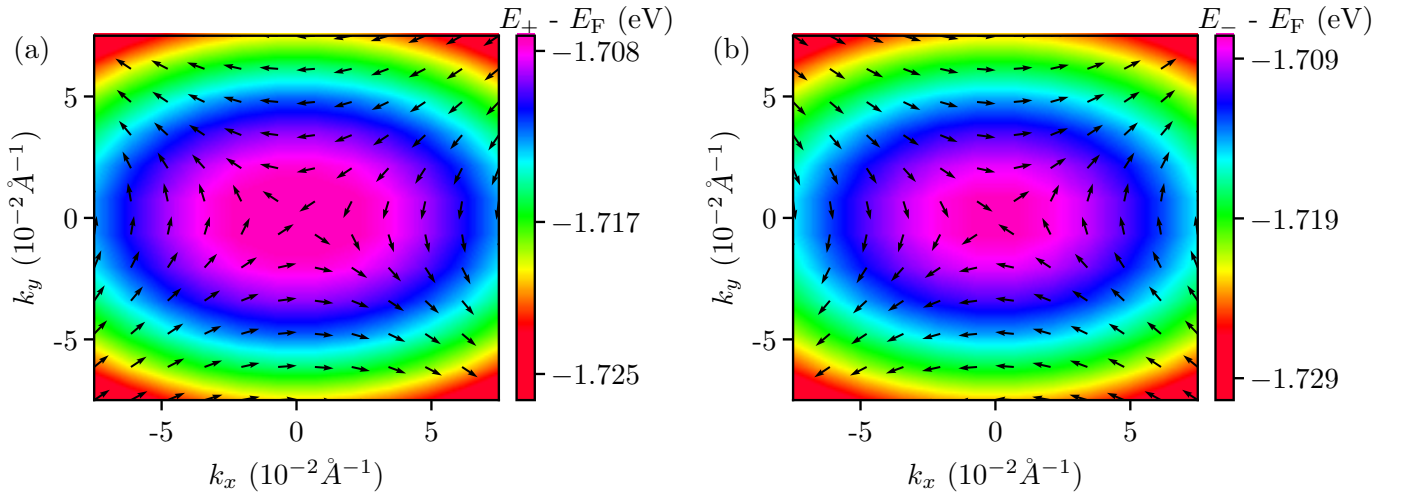


Figure S 14. Same as in Fig. S 10, but for the multilayer V/MgO(7MLs)/MoS₂.