

Supporting Information

For

Versatile Electronic Properties of Atomically Layered ScO_2

G.C. Loh ^{a,b*} and Ravindra Pandey ^{a*}

^aDepartment of Physics, Michigan Technological University, Houghton, Michigan 49931, USA

^bInstitute of High Performance Computing, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

A. Spin-Polarized Atom-Projected Band Structures of T- and H- ScO_2 Monolayers at different Hubbard U & J Parameters

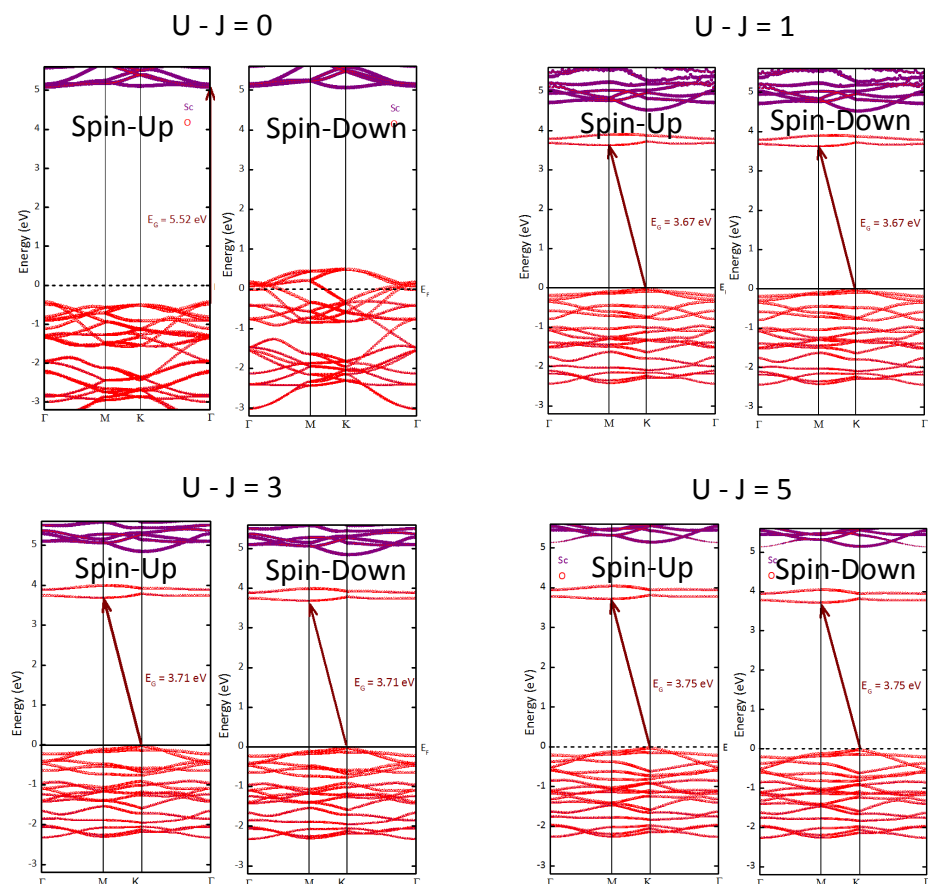


Figure S1. Spin-polarized atom-projected band structure of T-ScO₂ monolayer at different U-J parameters. The size of the data points indicates the spectral weight. Zero is taken to be Fermi energy.

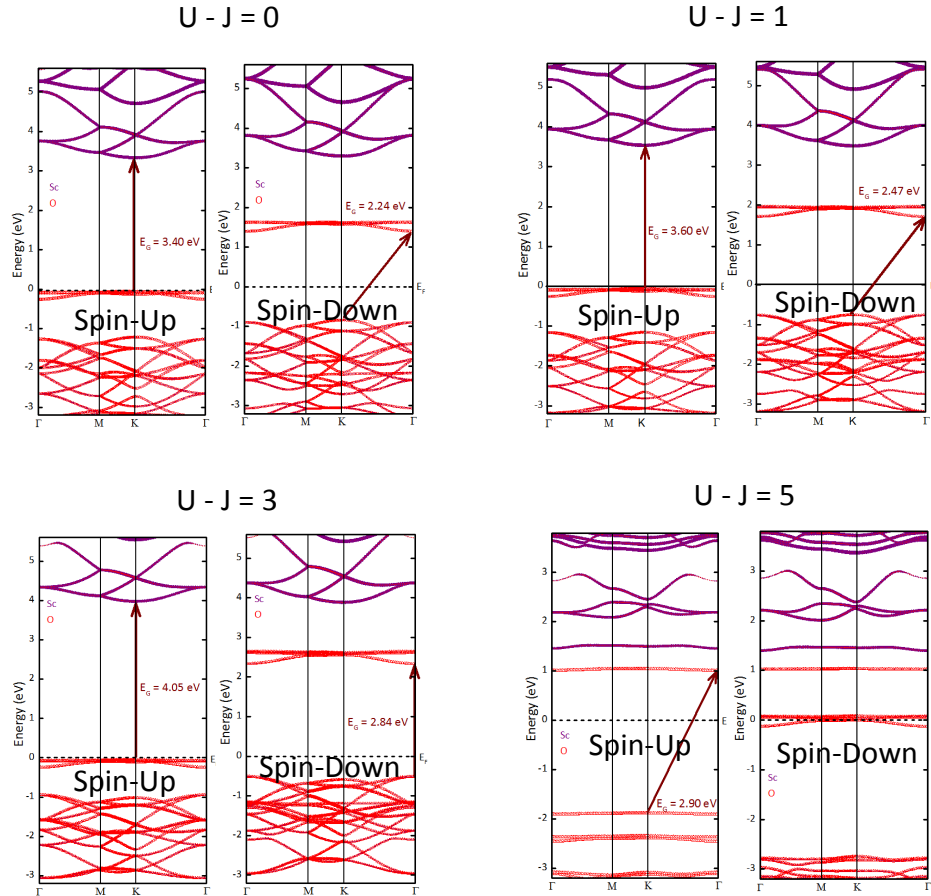


Figure S2. Spin-polarized atom-projected band structure of H-ScO₂ monolayer at different U-J parameters. The size of the data points indicates the spectral weight. Zero is taken to be Fermi energy.

B. Atom-Projected Band Structures of T-ScO₂ Monolayer, T-ScO₂ Bilayer, H-ScO₂ Monolayer & H-ScO₂ Monolayer

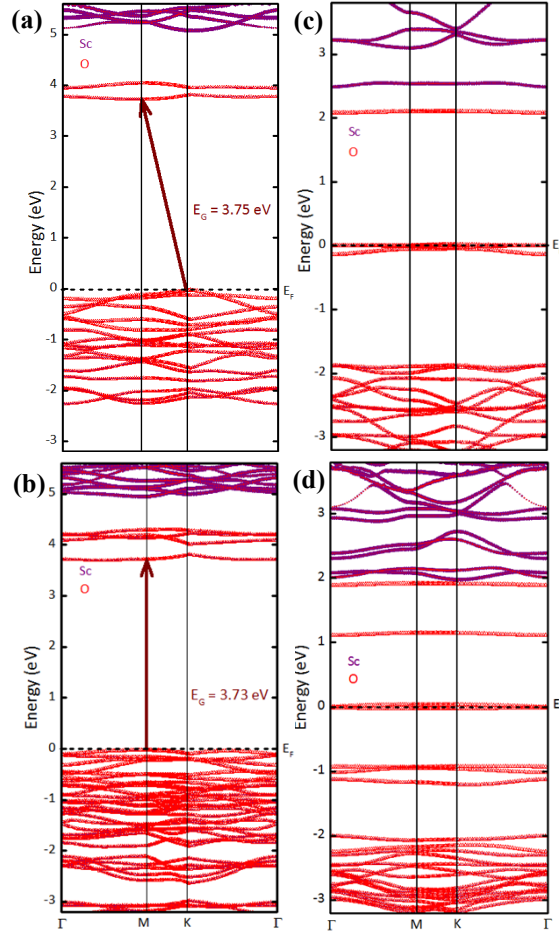


Figure S3. Atom-projected band structure of (a) T-ScO₂ monolayer, (b) T-ScO₂ bilayer, (c) H-ScO₂ monolayer, and (d) H-ScO₂ bilayer. Points in red and purple refer to contribution from Sc and O atoms, respectively. The size of the data points indicates the spectral weight. Zero is taken to be Fermi energy.

C. Orbital-Projected Band Structures of T-ScO₂ Monolayer, T-ScO₂ Bilayer, H-ScO₂ Monolayer & H-ScO₂ Monolayer

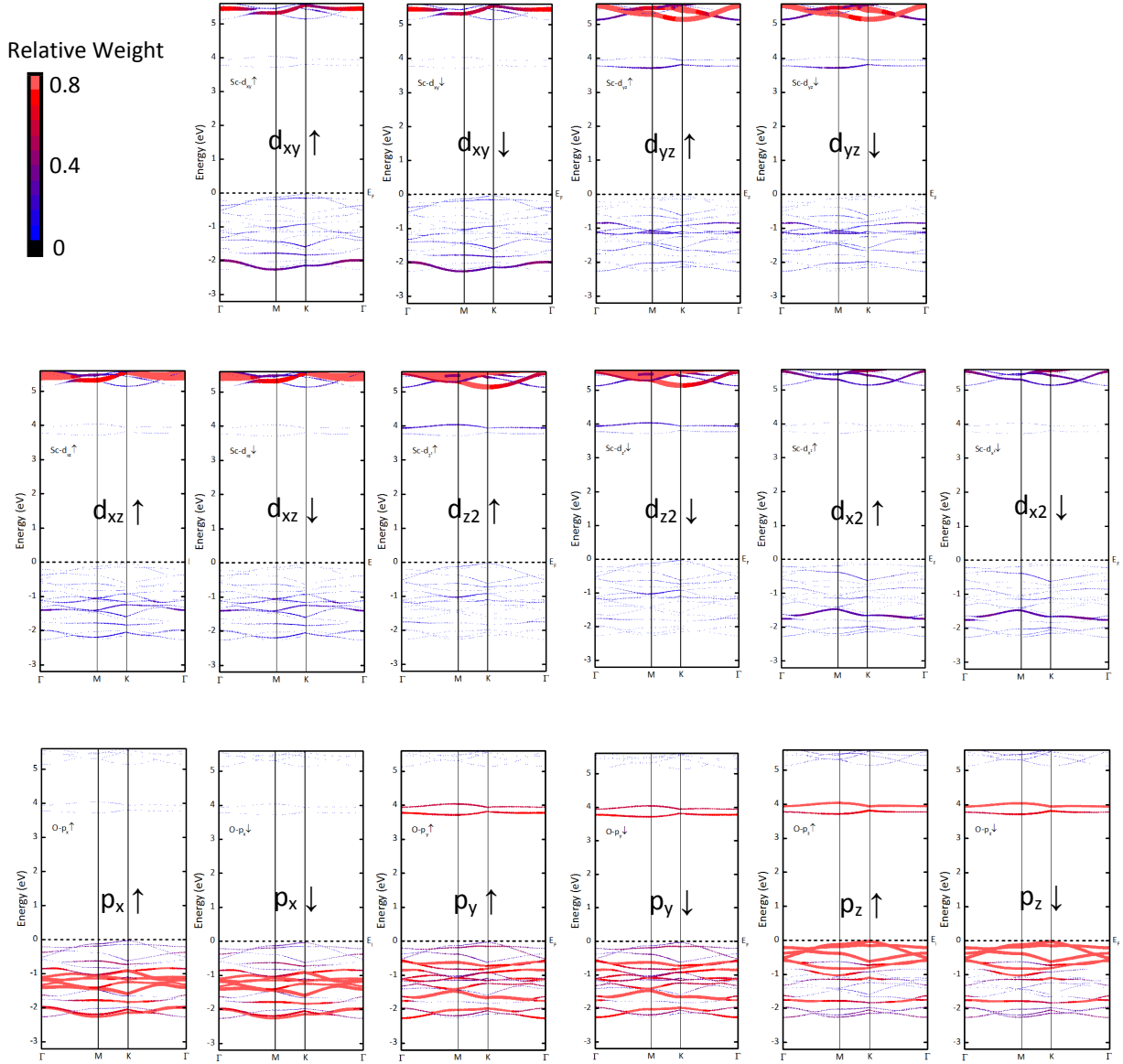


Figure S4. Orbital-projected band structure of T-ScO₂ monolayer. The size and color of the data points indicates the spectral weight. Zero is taken to be Fermi energy.

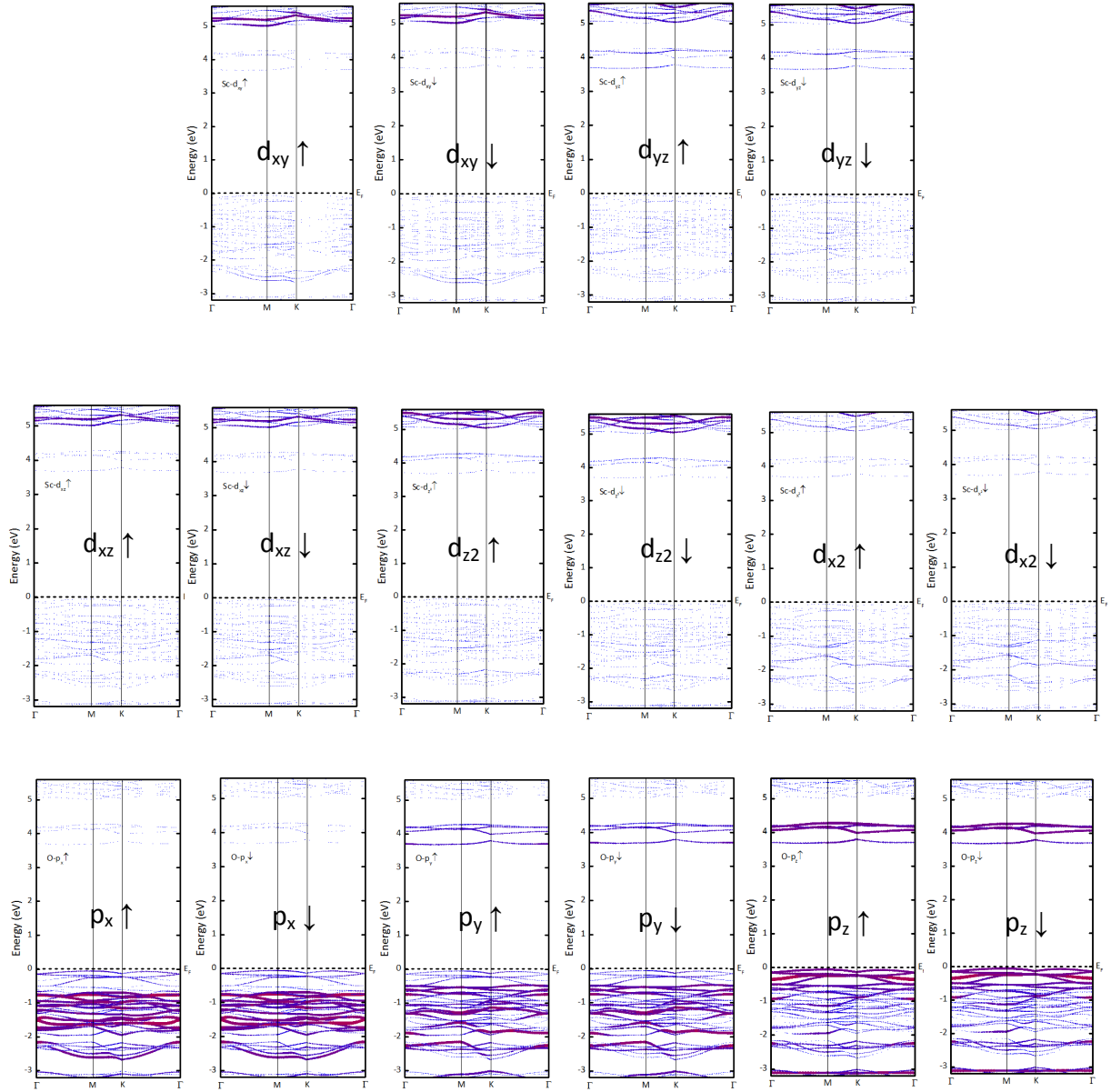


Figure S5. Orbital-projected band structure of T-ScO₂ bilayer. The size and color of the data points indicates the spectral weight. Zero is taken to be Fermi energy.

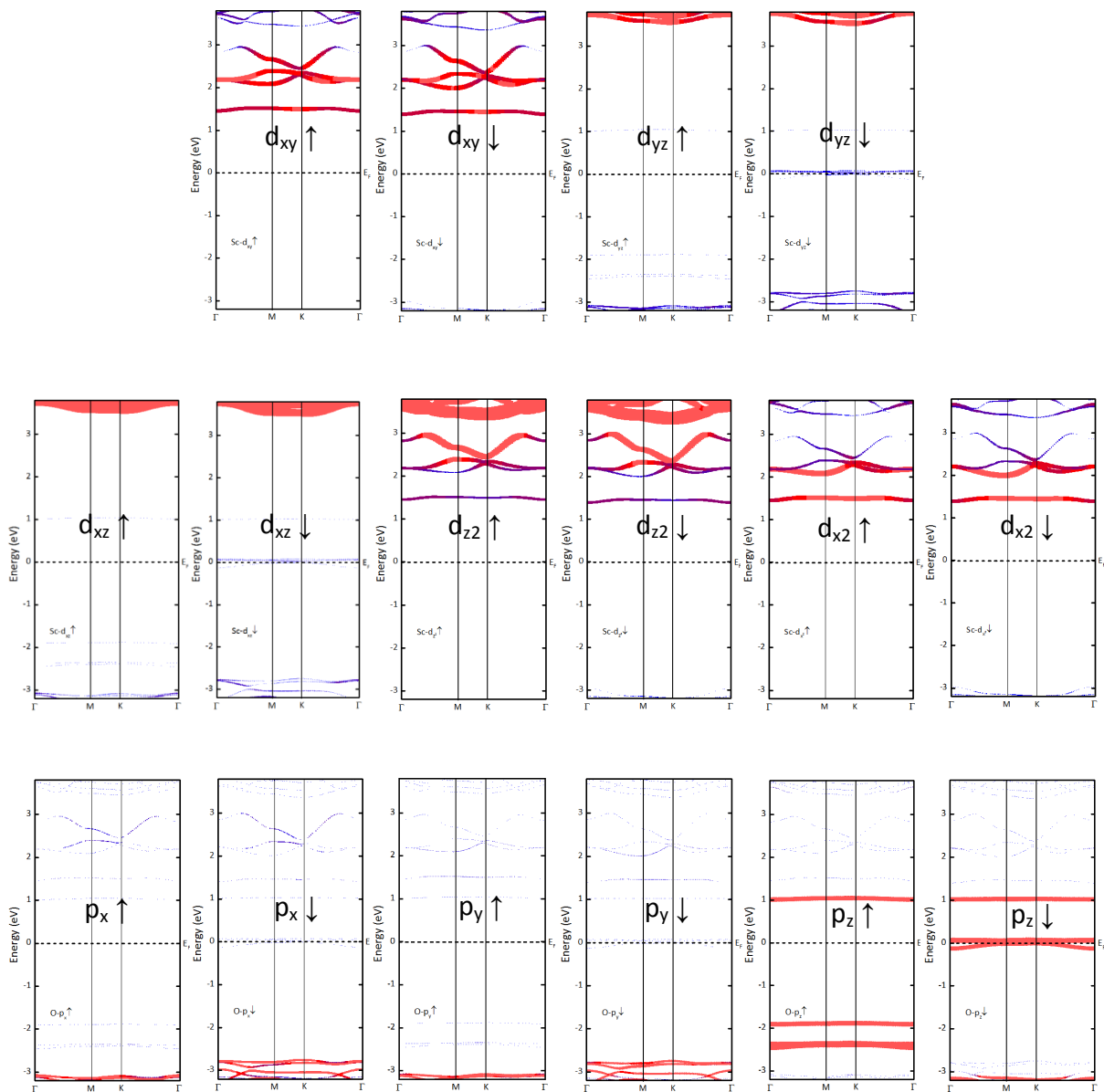


Figure S6. Orbital-projected band structure of H-ScO₂ monolayer. The size and color of the data points indicates the spectral weight. Zero is taken to be Fermi energy.

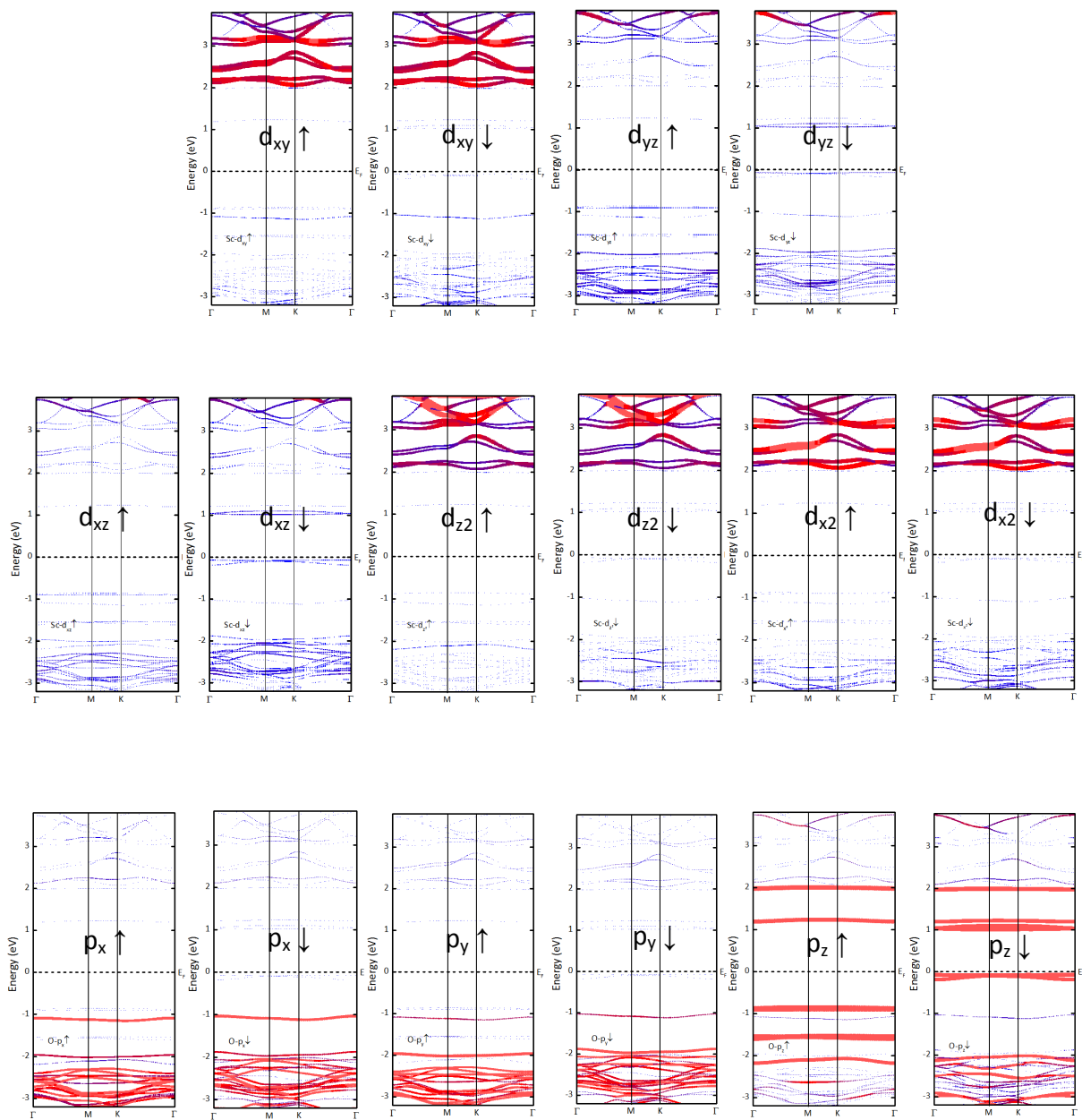


Figure S7. Orbital-projected band structure of H-ScO₂ bilayer. The size and color of the data points indicates the spectral weight. Zero is taken to be Fermi energy.

D. Laplacian of Charge Density

The Laplacian refers to the mathematical operator which is the second derivative or the trace of the Hessian of a function; it denotes the local minimum/maximum, or in other words, the saddle point of that function. Both minimum and maximum points are *critical points* at which the first derivatives of the function become zero. In the context of chemical topology, the differential operator reproduces the spherical shell structure of isolated atoms by alternating shells of charge concentration and shells of charge depletion. The outermost shell of charge concentration of an atom is called the valence shell charge concentration (VSCC), and its spherical symmetry is broken when the atom bonds with another atom. Another feature in the Laplacian plot of the electron density is the nuclear critical point (NCP), which is a local maximum in electron density, and is typically located at the position of a nucleus. A zero-flux surface contains a set of Laplacian trajectories which terminate at the bond critical point (bcp) where the Laplacian equals zero.

E. Evolution of Spin Density Distribution in H-ScO₂ Bilayer with Interlayer Separation

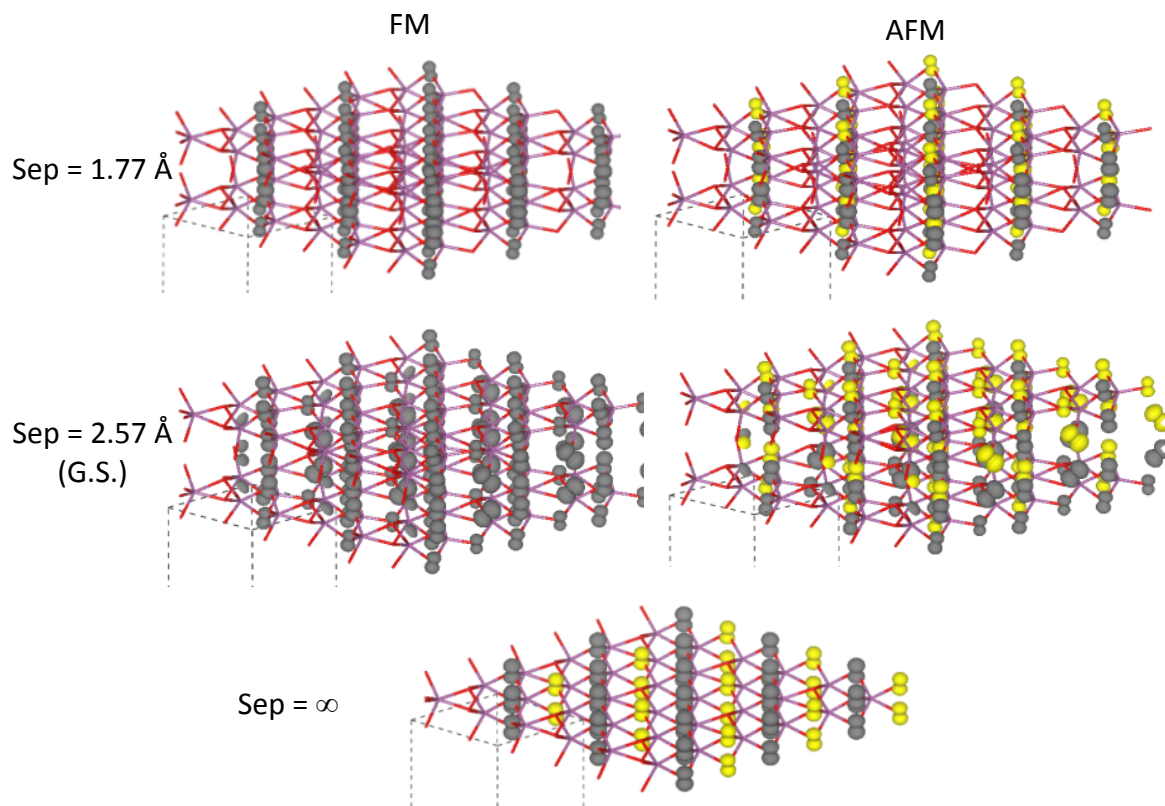


Figure S8. Evolution of spin density distribution in H-ScO₂ bilayer with interlayer separation in the FM and AFM spin configurations. The contour isovalue is $0.01 e/\text{Å}^3$. Regions in grey have a net spin-up density, whereas those in yellow have a net spin-down density.