

Supplementary Material (SM)

Symmetry-Driven Screening of Multifunctional 2D Monolayers with Valleytronic and Piezoelectric Properties: A High-Throughput Study

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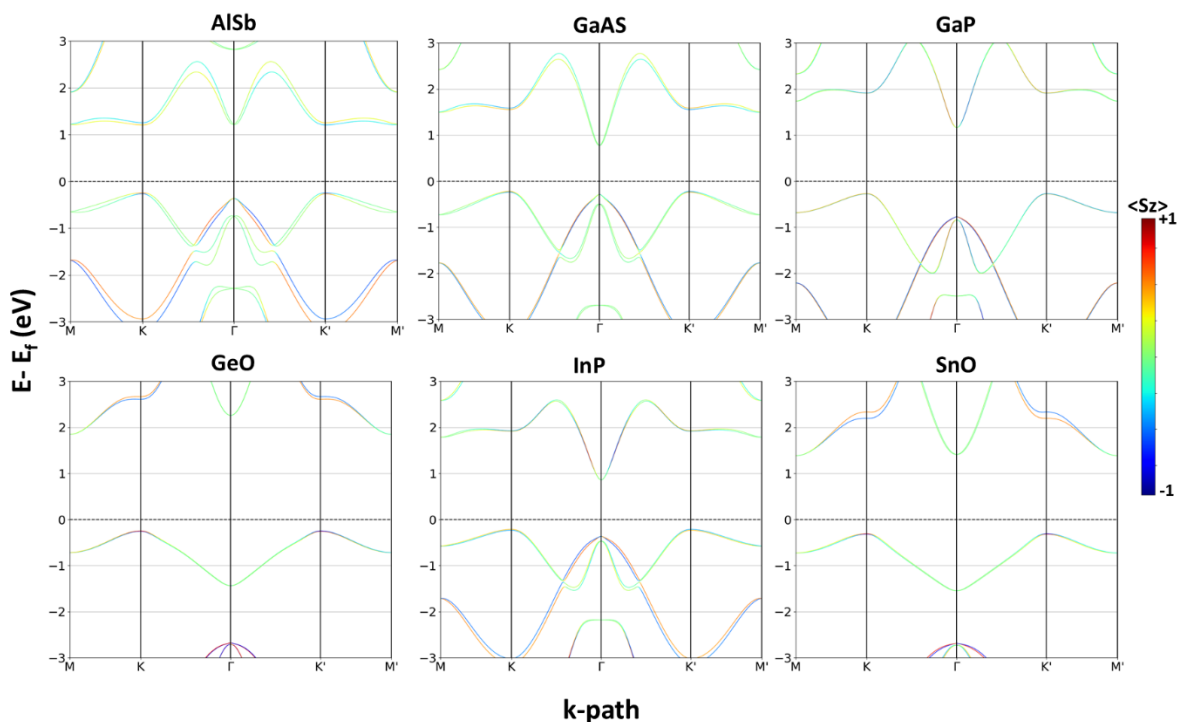


Figure S1(a). Spin projected (PBE+SOC) band structure corresponding to monolayers containing 2 atoms, in P3m1 space group.

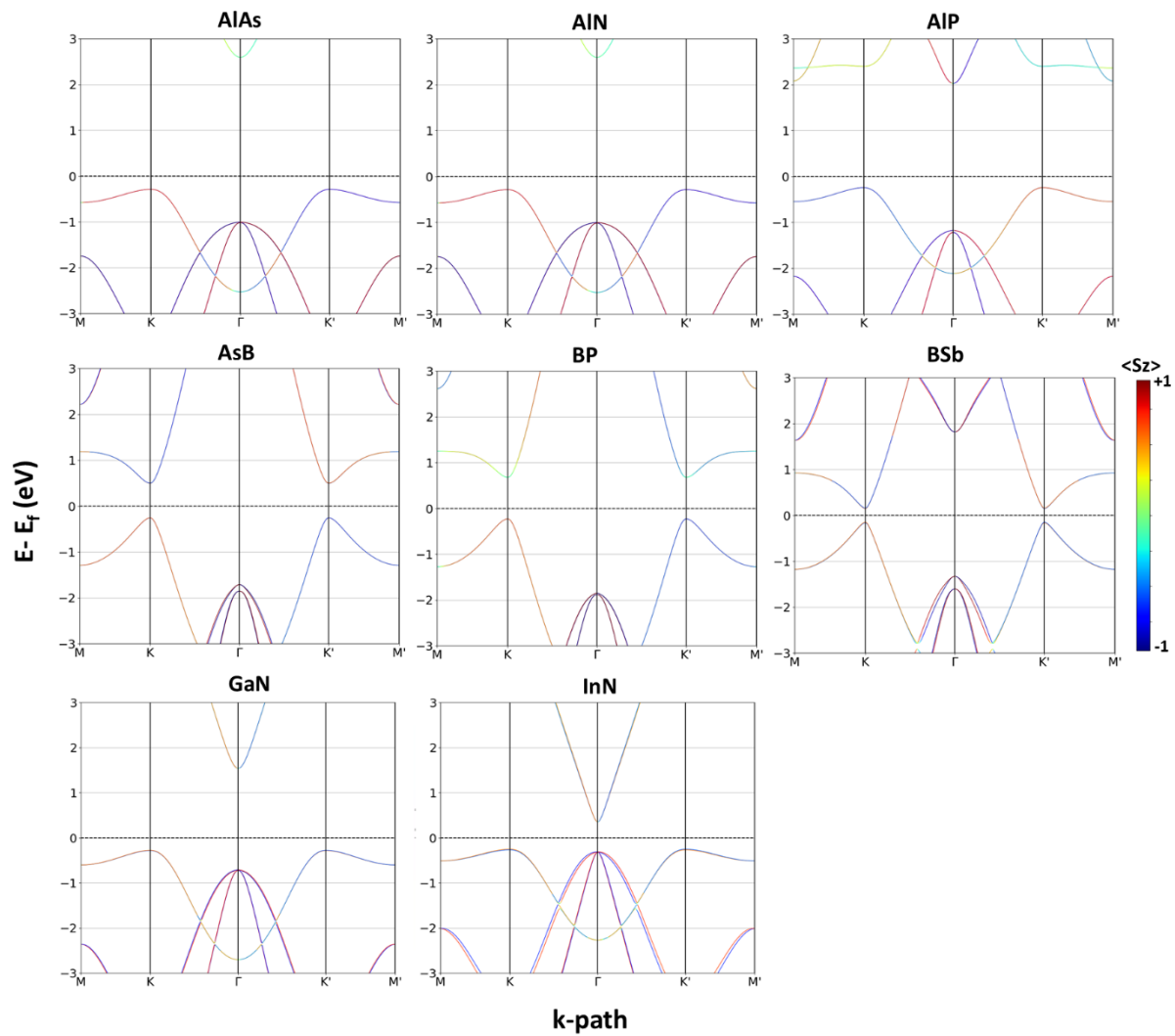


Figure S1(b). Spin projected (PBE+SOC) band structure corresponding to monolayers containing 2 atoms, in P-6m2 space group.

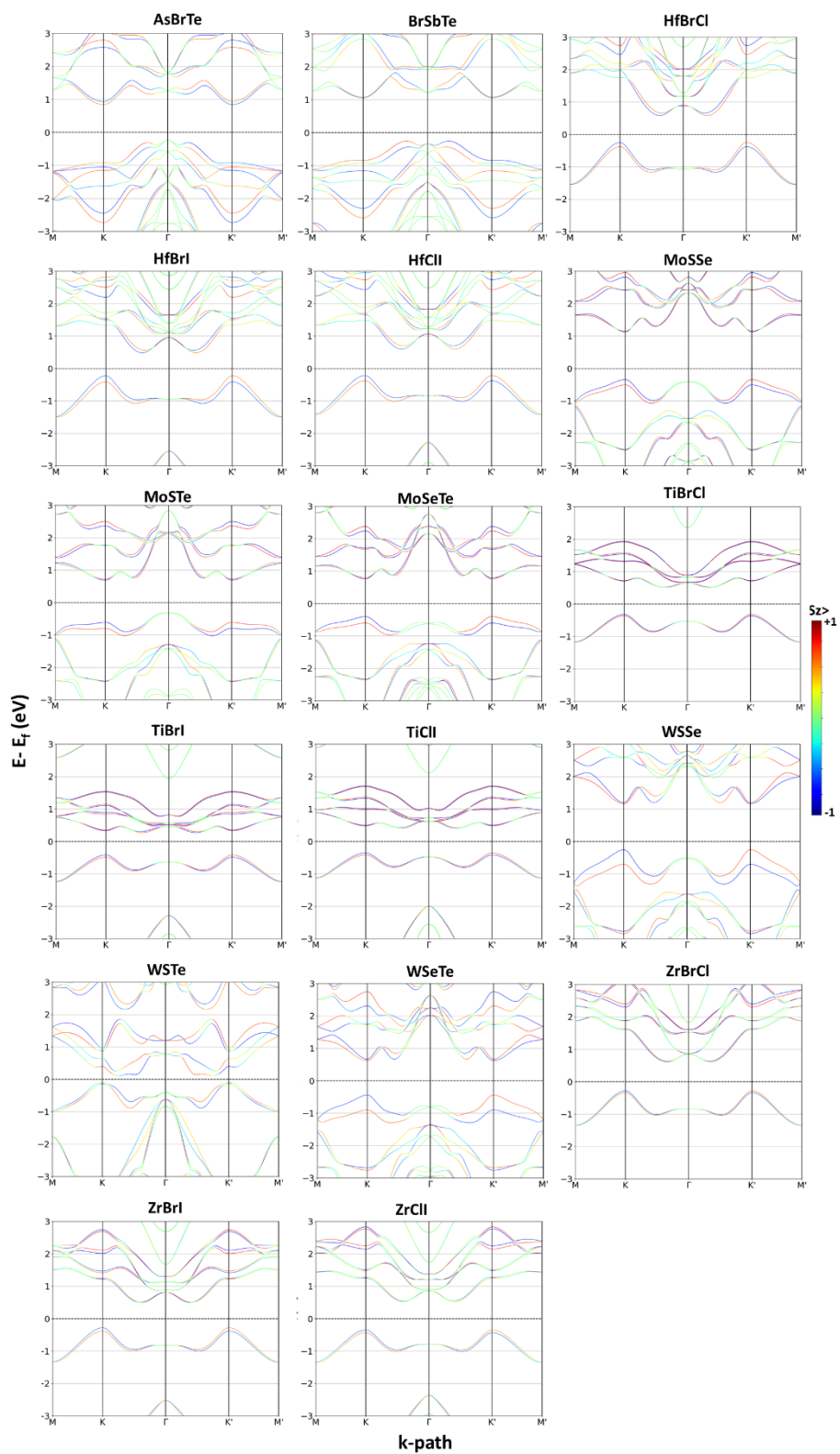


Figure S1(c). Spin projected (PBE+SOC) band structure corresponding to monolayers containing 3 atoms, in P-6m2 space group.

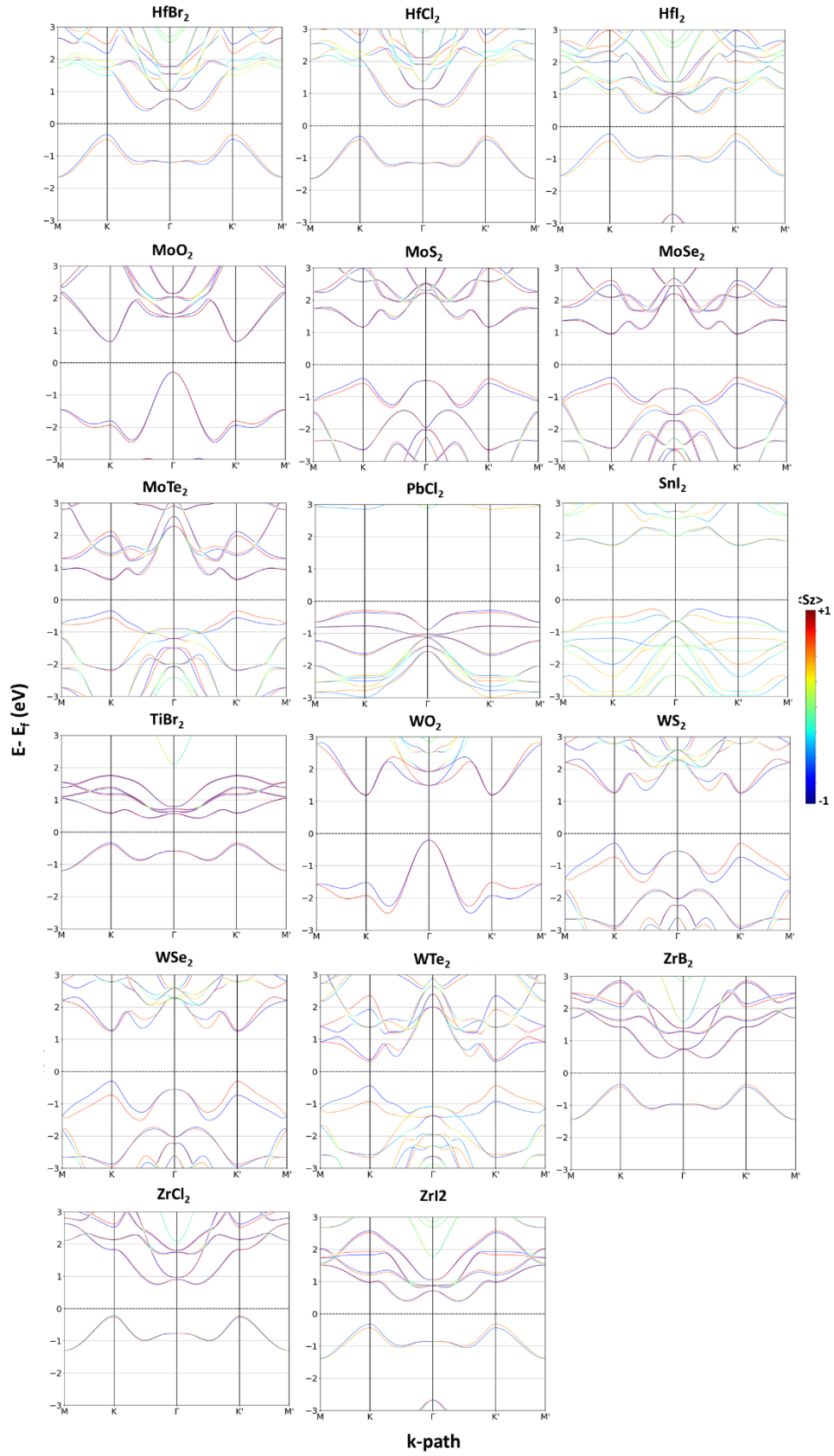


Figure S1(d). Spin projected (PBE+SOC) band structure corresponding to monolayers containing 3 atoms, in P-6m2 space group.

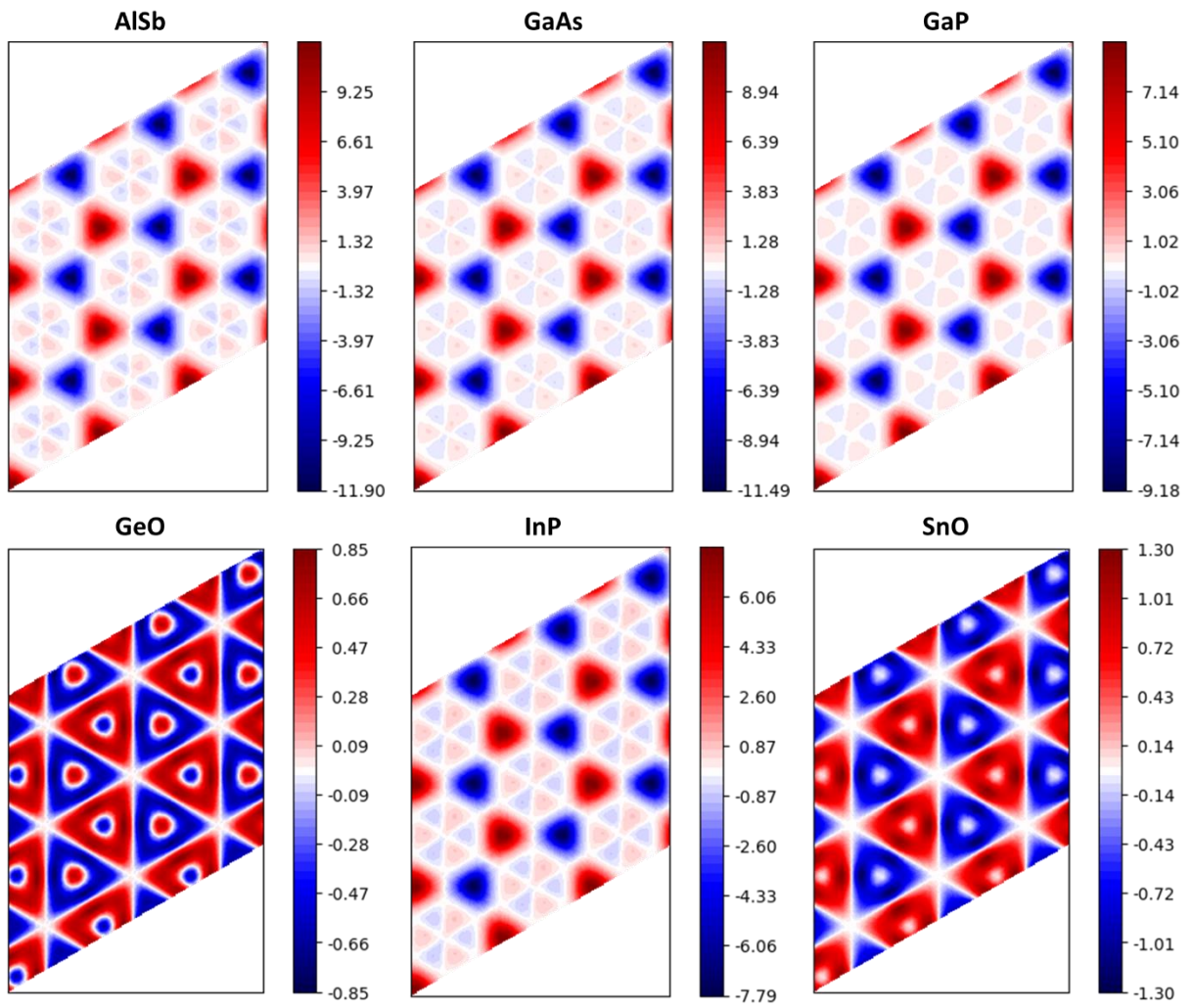


Figure S2(a). Contour plots of the Berry curvature distribution across the full BZ corresponding to monolayers containing 2 atoms, in P3m1 space group.

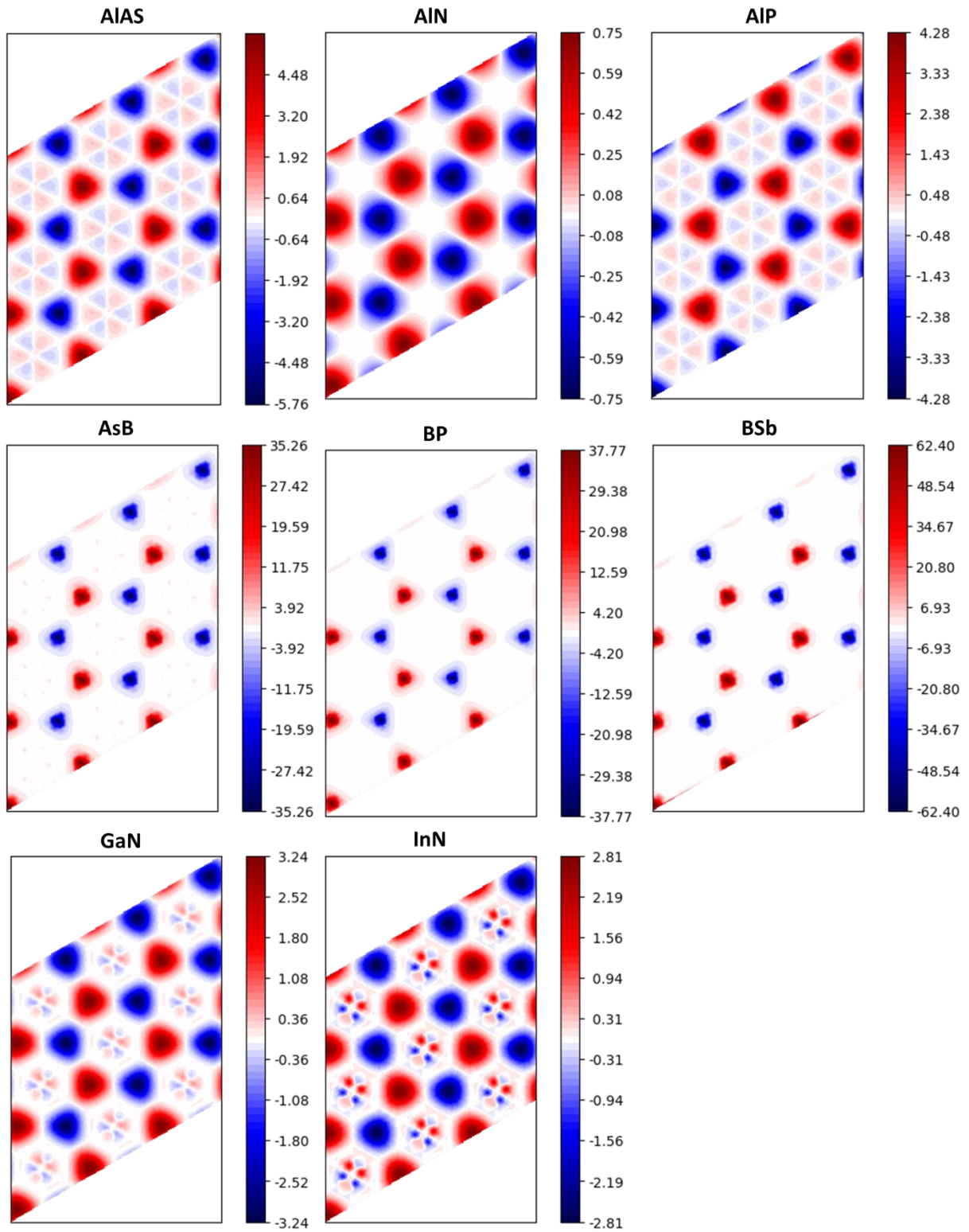


Figure S2(b). Contour plots of the Berry curvature distribution across the full BZ corresponding to monolayers containing 2 atoms, in P-6m2 space group.

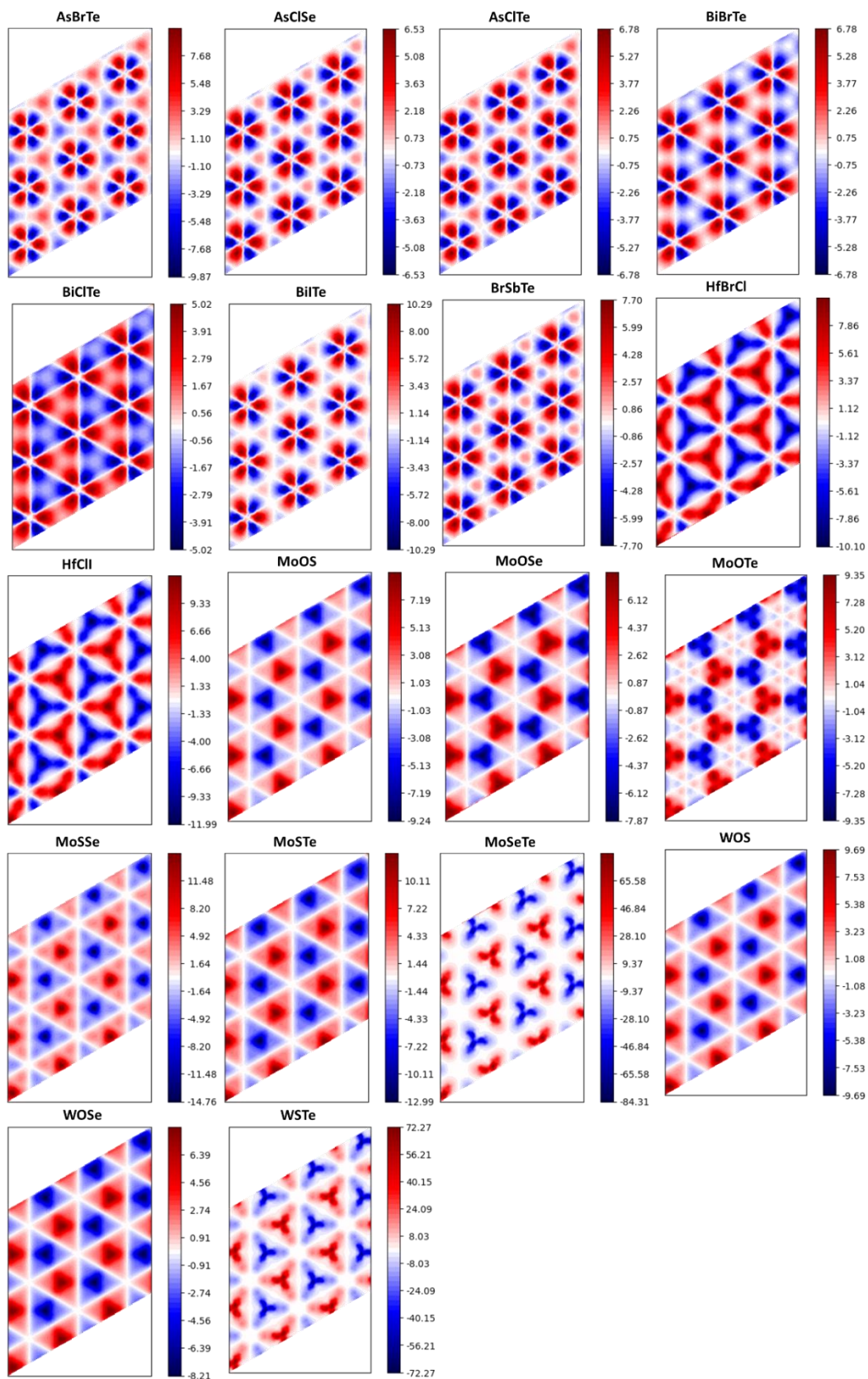


Figure S2(c) Contour plots of the Berry curvature distribution across the full BZ corresponding to monolayers containing 3 atoms, in P3m1 space group.

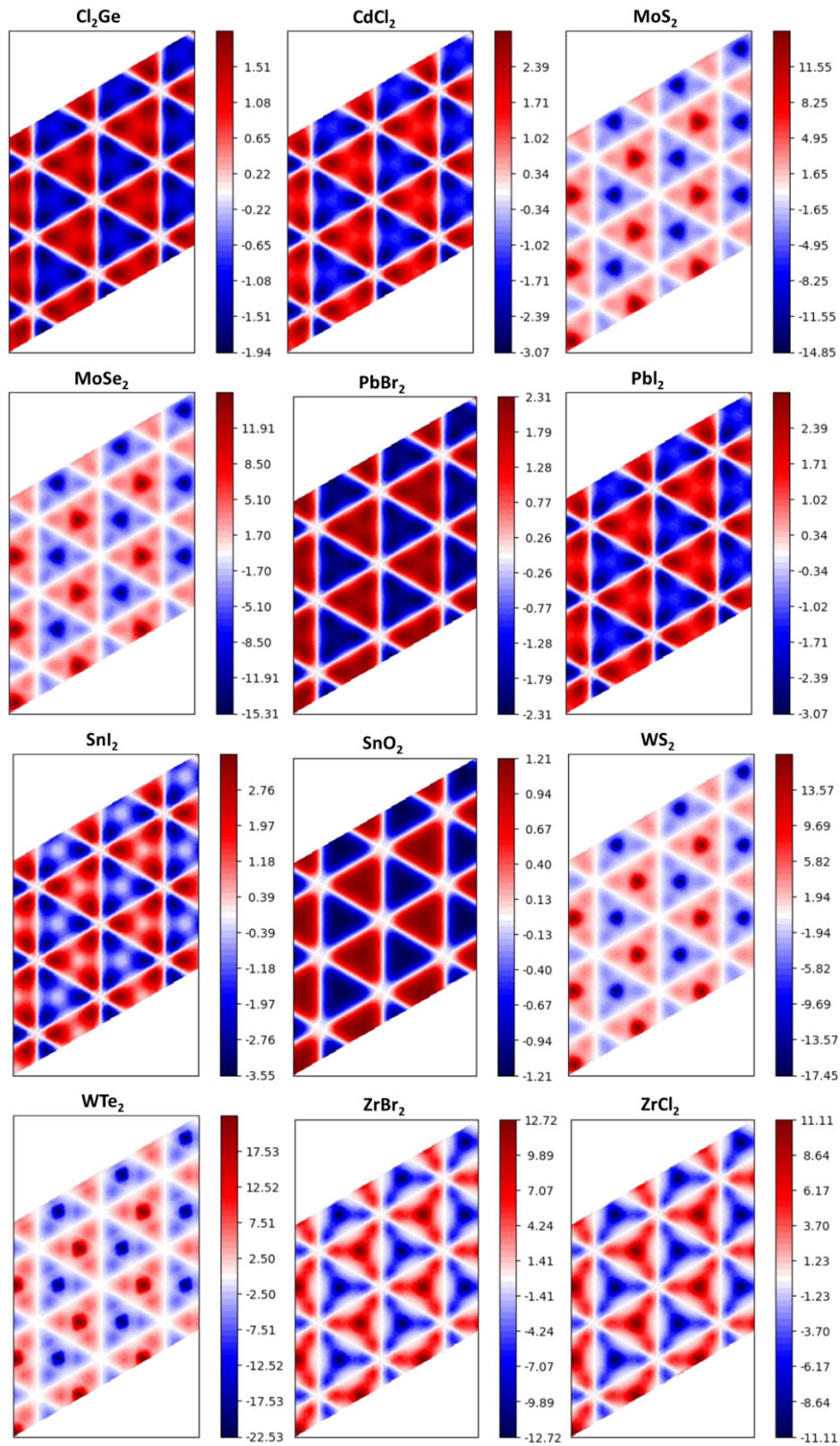


Figure S2(d). Contour plots of the Berry curvature distribution across the full BZ corresponding to monolayers containing 3 atoms, in P-6m2 space group.

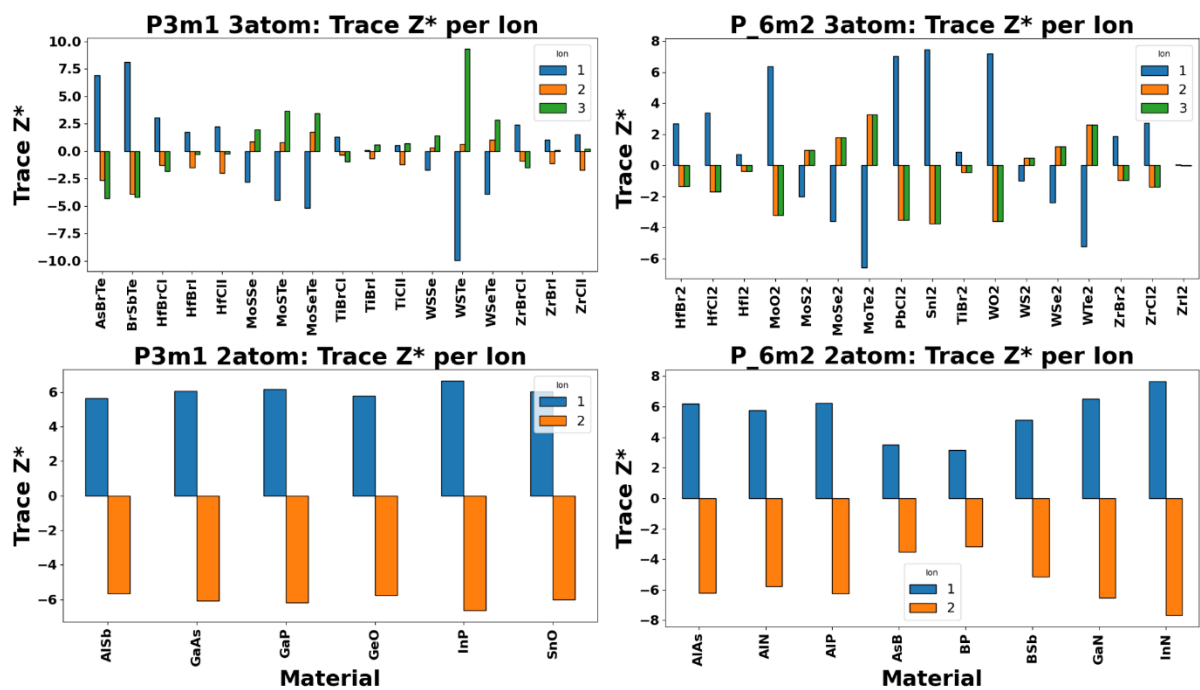


Figure S3: The trace of Born effective charge (Z^*) plotted for each material, the different colour bars represent the ions present in the monolayers.