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Electronic and magnetic engineering of transition metal dichalcogenides YOUJIAN TANG, VINCENT CRESPI, Penn State Univ. Physics Dept, VINCENT CRESPI GROUP TEAM — Transition metal dichalcogenides (TMDs) have moderate bandgaps and great potential in electronic and optoelectronic applications. We show that by intercalation and compensated doping of transition metal ions, we could generate a "half-semiconductor", half-metal or doped magnetic semiconductor. We will also show that covalently connecting a single layer of WS2 to a small aromatic molecule with appropriate electronegativity, it is possible to align the molecular energy levels with the WS2 conduction band edge, yielding an electronic structure of potential interest for thermoelectric applications, and covalently connecting single-layer WS2 to magnetic coordination compounds could introduce magnetization into the WS2 layer.

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