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Layer-dependent Magnetism and Non-trivial Topology of Monolayer and Bilayers ReX_3 (X = Br, I). SHARAD MAHATARA, BORIS KIEFER, New Mexico State University — Two-dimensional (2D) van der Waals (vdW) magnets such as transition metals (TM) halides exhibiting topological states have provided a fertile ground for spintronic and quantum computing applications. In TM halides the presence of topologically protected states depends on the delicate balance of near degenerate interactions: (1) magnetic exchange interaction, (2) interlayer vdW interactions, and (3) amplified spin-orbit coupling (SOC). In this contribution, we have computed electronic, magnetic and topological properties of 2D (mono- and bi-layers) of ReX_3 (X = Br, I) by DFT and self-consistent DFT-Hubbard-U including vdW interactions and SOC. We report for the first-time layer-dependent magnetism in ReX_3 (X = Br, I). Furthermore, our results predict that topologically protected quantum states vanish if Hubbard-U is used to improve the description of the electronic structure description of these materials. Therefore, additional biases are necessary to facilitate the formation of time-reversal broken topologically protected states with expected favorable long qubit decoherence times for performance improved quantum computers.

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