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Molecular j_{eff} states in ternary transition metal chalcogenides AM_4X_8 ¹ HEUNG-SIK KIM, Department of Physics, Korean Advanced Institute of Science and Technology, Daejun 305-701, Korea, JINO IM, Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208, USA, MYUNG JOON HAN, Department of Physics, Korean Advanced Institute of Science and Technology, Daejun 305-701, Korea, HOSUB JIN, Center for Correlated Electron Systems, Institute for Basic Science / Department of Physics and Astronomy, Seoul National University, Seoul 151-747, K — Spin-orbit-coupling(SOC)-induced j_{eff} states, reported in several iridium oxide compounds, is the key ingredient in understanding the interesting cooperation between SOC and the electron correlations. From our density functional theory calculations we suggest that, a series of ternary transition metal chalcogenides AM_4X_8 ($A = \text{Ga}$, $M = 4d$ and $5d$ transition metal atoms, $X = \text{chalcogen atoms}$) host the j_{eff} states in a molecular form. Wide range of the bandwidth covered with the external or chemical pressure enable one to access a broad range of electron correlation strength in a single compound. Implications of our results in both the weak and strong coupling regime are discussed. Our finding provides an ideal playground in exploring the j_{eff} physics and the resulting emergent phenomena.

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