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Density Functional and Effective Hamiltonian Calculations of the Spin-Orbit Coupling in WS_2 Monolayers MOHAMMAD MAHDI VALIZADEH, SHANAVAS VEEDU, SASHI SATPATHY, University of Missouri - Columbia — The monolayer metal dichalcogenides such as MoS_2 and WS_2 are currently an emerging class of 2D materials owing to their possible applications in 2D electronics including spintronics. The spin-orbit interaction coupled with broken structural inversion symmetry or external electric field, can give rise to interesting effects such as Rashba spin splitting. With the help of density functional theory based electronic structure calculations and tight binding Hamiltonian based models, we study the effect of an external electric field in monolayers of high-Z dichalcogenide WS_2. Density functional calculations predict strong spin-orbit coupling with a large Zeeman like splitting at the K-point in the H-structure, even in the absence of any external field. We also find Rashba splitting of bands at Γ point close to the Fermi level which can be tuned using the applied electric field. Based on the DFT calculations, we derive an effective Hamiltonian for this system which offers a simple model to understand the interplay of spin-orbit and electric fields in this system.

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