Band nesting, massive Dirac Fermions and valley Lande and Zeeman effects in transition metal dichalcogenides

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We describe here the electronic properties of 2D transition metal dichalcogenide crystals using ab–initio and tight binding methods. We discuss the origin of band nesting resulting from Q points in the Brillouin zone [1] and derive the two band effective massive Dirac Fermion model. The model allows us to introduce the magnetic field, obtain Landau levels and describe Zeeman and Lande effects in the two nonequivalent valleys.

Our approach builds on previous theoretical works as well as our new ab–initio results allowing us to develop the simplest tight binding model which captures the physics of TMDCs and allows the application of magnetic field. The wave function is constructed out of orbitals localized on metal atoms and sulfur dimmers. Guided by ab–initio calculations, we choose basis consisting of symmetric d orbitals with quantum numbers $l = 2$ and $m_d = \pm 2, 0$ and dimer p orbitals with $l = 1$ and $m_p = \pm 1, 0$. We derive explicit form of the metal nearest neighbor sulfur dimer tunneling matrix elements at $+K$, $-K$ and Γ points and include next nearest neighbor metal-metal atom tunneling perturbatively. The matrix elements of the effective 6*6 tunneling Hamiltonian are fitted to band structure calculated using first-principles methods. The origin of the Q point minima in the conduction band paired with K point minima are traced to the interaction of different metal orbitals at K and Γ points. The calculated joint density of states shows maxima corresponding to transitions into the Q point minima. For energies and wavevectors close to the K points we derive an effective two band massive Dirac Fermion model. We calculate the Landau levels and show the existence of valley Zeeman and valley Lande effect in agreement with recently measured valley Zeeman factors in MoS_2 [2]. We next discuss the role of Coulomb interactions on the optical transitions in TMDCs.

[1] Kadantsev, E. S., Hawrylak, P., *Solid State Communications* **152**, 909 (2012).
[2] Stier, A. V., McCreary, K. M., Jonker, B. T., Kono, J., Crooker, S. A., *Nature Comm.* **7**, 10643 (2016)