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A Tight Binding Approach to Strain in Monolayer Transition-Metal Dichalcogenides ALEXANDER PEARCE, GUIDO BURKARD, University of Konstanz, Germany — We present a model of the electronic properties of the monolayer transition-metal dichalcogenides based on a tight binding approach which includes the effects of strain and curvature of the crystal lattice. Mechanical deformations of the lattice change bond lengths leading directly to corrections in the electronic Hamiltonian, while curvature of the crystal lattice mixes the orbital structure of the electronic Bloch bands. We first present an effective low energy Hamiltonian describing the electronic properties near the K point in the Brillouin zone, then present the corrections to this Hamiltonian due to arbitrary mechanical deformations and curvature in a way which treats both effects on an equal footing. This analysis finds that local area variations of the lattice allow for tuning of the band gap and effective masses, where the application of uniaxial strain decreases the magnitude of the direct band gap at the K point. Additionally, strain induced bond length modifications create a fictitious gauge field but with a coupling that is smaller than seen in related materials like graphene. Whereas curvature of the lattice leads to appearance of both an effective in-plane magnetic field which couples to spin degrees of freedom and a Rashba-like spin-orbit coupling.

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