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Charge-Density Wave Driven Phase Transitions in Single-Layer MoS_2 HOULONG L. ZHUANG, Department of Materials Science and Engineering, Cornell University, MICHELLE D. JOHANNES, Center for Computational Materials Science, Naval Research Laboratory; Department of Materials Science and Engineering, Cornell University, RICHARD G. HENNIG, Department of Materials Science and Engineering, Cornell University — Phase transitions in single-layer MoS_2 are frequently observed in experiments. We reveal that charge doping can induce the phase transition of single-layer MoS_2 from the $2H$ to the $1T$ structure. Further, the $1T$ structure undergoes a second phase transition due to the occurrence of a charge-density wave (CDW). By comparing the energies of several possible resulting CDW structures, we find that the $\sqrt{3}a \times a$ orthorhombic structure is the most stable one, consistent with experimental observations. Moreover, we discover that the band structure of the $\sqrt{3}a \times a$ structure possesses a Dirac cone, which is split by spin-orbit interactions into a bandgap of 50 meV. We show that the underlying CDW transition mechanism is not electronic, but can be controlled by charge doping nonetheless. Finally, we calculate the interface energy and band offsets of a lateral heterostructure formed by the $2H$ and $\sqrt{3}a \times a$ structures.

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