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Tuning the Electronic and Chemical Properties of Monolayer MoS_2 Adsorbed on Transition Metal Substrates[1] WEI CHEN, University of Tennessee, ELTON SANTOS, Harvard University, WENGUANG ZHU, University of Science and Technology of China, EFTHIMIOS KAXIRAS, Harvard University, ZHENYU ZHANG, University of Science and Technology of China — Using first-principles calculations within density functional theory, we investigate the electronic and chemical properties of a single-layer MoS_2 adsorbed on Ir(111), Pd(111), or Ru(0001), three representative transition metal substrates having varying work functions but each with minimal lattice mismatch with the MoS_2 overlayer. We find that for each of the metal substrates, the contact nature is of Schottky type, and the dependence of the barrier height on the work function exhibits a partial Fermi-level pinning picture. Using hydrogen adsorption as a testing example, we further demonstrate that the introduction of a metal substrate can substantially alter the chemical reactivity of the adsorbed MoS_2 layer. The enhanced binding of hydrogen, by as much as about 0.4 eV, is attributed in part to a stronger H-S coupling enabled by the transferred charge from the substrate to the MoS_2 overlayer, and in part to a stronger MoS_2-metal interface by the hydrogen adsorption. These findings may prove to be instrumental in future design of MoS_2-based electronics, as well as in exploring novel catalysts for hydrogen production and related chemical processes.

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