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Chemically-exfoliated single-layer MoS_2: stability, lattice dynamics and catalytic adsorption from first principles MATTEO CALANDRA, CNRS and Université P. et M. Curie — Chemically and mechanically exfoliated MoS_2 single-layer samples have substantially different properties. While mechanically exfoliated single-layers are mono-phase (1H polytype with Mo in trigonal prismatic coordination), the chemically exfoliated samples show coexistence of three different phases, 1H, 1T (Mo in octahedral coordination) and $1T^{'}$ (a distorted 2×1 1T-superstructure). By using first-principles calculations, we investigate the energetics and the dynamical stability of the three phases. We show that the 1H phase is the most stable one, while the metallic 1T phase, strongly unstable, undergoes a phase transition towards a metastable and insulating $1T^{'}$ structure composed of separated zig-zag chains. We calculate electronic structure, phonon dispersion, Raman frequencies and intensities for the $1T^{'}$ structure. We provide a microscopical description of the J_1, J_2 and J_3 Raman features first detected more then 20 years ago, but unexplained up to now. Finally, we show that H adsorbates, that are naturally present at the end of the chemical exfoliation process, stabilize the $1T'$ over the 1H one.

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