Abstract Submitted
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Structure change, layer sliding, and metallization in high-pressure MoS2[1] ERIO TOSATTI, SISSA, ICTP, CNR-IOM Democritos, LILIANA HROMADOVA, ROMAN MARTONAK, Comenius University Bratislava — Based on ab initio calculations and metadynamics simulations, we predict that 2H-MoS_2, a layered insulator, will metallize under pressures in excess of 20-30 GPa. In the same pressure range, simulations and enthalpy optimization predict a structural transition. Reminiscent of this material's frictional properties, free mutual sliding of layers takes place at this transition, where the original $2H_c$ stacking changes to a $2H_a$ stacking typical of 2H-$NbSe_2$, a transformation which explains for the first time previously mysterious X-ray diffraction data. Phonon and electron phonon calculations suggest that metallic pristine MoS_2 will require ultrahigh pressures in order to develop superconductivity.

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Erio Tosatti
SISSA, ICTP, CNR-IOM Democritos

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