

## Abstract:

The structure of MoS<sub>2</sub> with strong covalent bonds in plane and weak van der Waals interactions out of plane gives rise to interesting properties for applications such as solid lubricants, optoelectronics, sensors, and electrochemical devices. Transition metal doping is found to improve the performance in tribology [MR Vazirisereshk et al., *Lubricants* 7, 57 (2019)] and hydrodesulfurization. We study the structure and properties of Ni-doped MoS<sub>2</sub> in the 1H and 1T monolayer and 2H and 3R bulk polytypes, using density functional theory (DFT). We calculated the formation energy of Ni at different sites (Mo and S substitution, intercalation/adsorption) to identify the most energetically favorable ones, and analyzed the energy for layer separation and the energetics of interlayer sliding. We studied the effect of Ni doping on local bonding and lattice structure at different dopant concentrations to assess possible phase changes. This work gives insight into the previously unclear structure, properties, and solid lubrication performance of Ni-doped MoS<sub>2</sub>.