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First Principles Study of Monolayer MoS_2 with Defects and Vacancy YINGYE GAN, HUIJUAN ZHAO, Clemson Univ — Unlike graphene and silicene, monolayer molybdenum disulfide (MoS_2) is a direct band gap transition metal with interesting electrical, mechanical, and optical properties. As a potential material in NEMS application, it is necessary to systematically study the defect effects to the material properties of MoS_2 under strain tuning. We will perform ab initio density functional theory based calculations to study the mechanical and electronic property variation of MoS_2 with different vacancy types and vacancy densities, such as Young's modulus, Poisson's ratio, fracture strength and band gap. The failure mechanism under various strain conditions will be investigated through the phonon dispersion curves. We expect to elucidate the relation between material properties of MoS_2 with strain tuning and defect tuning.

Huijuan Zhao
Clemson Univ

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