Abstract Submitted
for the CUWIP22 Meeting of
The American Physical Society

Two-Dimensional Sliding of Ni-Doped MoS2 ELSA VAZQUEZ, ENRIQUE GUERRERO, DAVID A. STRUBBE, University of California, Merced, SAIL TEAM[1] — MoS_2 is a layered transition-metal dichalcogenide shown to have many functional properties, but an original application is lubrication, especially for outer space. Ni is a dopant known to increase its lubricity. In this computational study, we slide in the x and y directions the bi-layers of Ni-doped MoS_2 and use density-functional theory to find the sliding potential energy surface (PES) in a 2×2 supercell. The structure is doped by swapping a Mo or S atom and by intercalation where we insert Ni between the layers leading to octahedral or tetrahedral structures. For the two substitution sites, there are overall differences in magnitudes. The tetrahedral site has the largest amplitude with steep paths between saddle points. The octahedral site has smoother transitions between stable and unstable sites. Compared to the PES of the pristine cell there is a resemblance for the substituted sites, but not for the intercalated sites. The Mo-substituted supercell roughly shares with pristine the positions corresponding to the stable, metastable, and unstable sites. Notably, the S-substituted case seems to switch the positions of the stable and meta-stable sites. Our findings on the sliding potential of Ni-doped MoS_2 provide insights into its mechanisms for lubrication.

[1]SAIL is the Srubbe Ab Initio Laboratory

Elsa Vazquez
University of California, Merced

Date submitted: 11 Jan 2022 Electronic form version 1.4