

A model for the temperature-dependence of the friction in MoS<sub>2</sub> has been developed which relies upon the heights of energy barriers to characterize the molecular pathways of MoS<sub>2</sub>-flake sliding . Here we present atomistic calculations that show changes to these barriers in the presence of water and oxygen, two major environmental contaminants affecting the friction. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.