

A model for the temperature-dependence of the friction in MoS₂ has been developed which relies upon the heights of energy barriers to characterize the molecular pathways of MoS₂-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.