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Predicting Tribochemically Induced Reactions of MoS_2

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Abstract

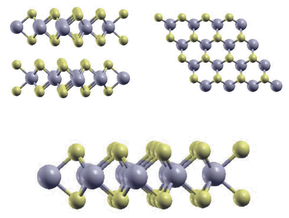
We investigate how local surface strains influence the evolution of the frictional properties of MoS_2 while simultaneously examining the change in reactivity induced by surface strain and applied loads. This will give insight into properties such as reduction and oxidation potentials. As a 2-D material is deformed, changes in the local bond-order should render specific locations more susceptible to tribochemical reactions.

The nature of tribochemical reactions is still vague, thus we used atomistic simulation to construct models that accurately predict results from tribological experiments. Establishing relationships between the properties of MoS_2 and frictional performance aids in developing more robust experimental studies and helps to better understand friction, wear, and lubrication.

Introduction

Tribology is the study of friction and wear at interacting surfaces. The impact of friction and wear on the global economy is directly related to energy loss in systems and how that energy may be recovered to reduce fuel consumption. Ref1 indicated that utilizing new surfaces, materials and lubrication technologies for friction reduction and wear protection in vehicles and other machinery worldwide could realize a long-term savings of 1.4 percent of annual GDP and 8.7 percent of total energy consumption. Molybdenum disulfide (MoS_2) has been an integral part of material technologies used to control friction and wear in applications.

Ref1: Holmberg, K. et al., Friction 2017 5, 263-264



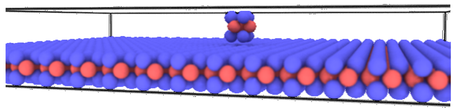
Ahmad, S. and Mukherjee, S. (2014) A Comparative Study of Electronic Properties of Bulk MoS2 and Its Monolayer Using DFT Technique: Application of Mechanical Strain on MoS2 Monolayer. *Graphene*, **3**, 52-59.

MoS_2 is a transition metal dichalcogenide that is useful in solid lubrication, heterostructures, catalysis and 2-D-based electronic devices. The lamellar structure of MoS2 is similar to that of graphene, mica and hexagonal boron nitride, with weak interactions between the lamella leading to exceptional frictional properties. This leads to the need to understand the interactions at the atomic scale. Uncovering the physics of atomic-scale friction and its influence on energetics during sliding is of value in a fundamental understanding.

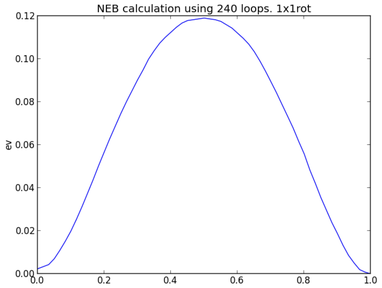
Methodology

- A blend of molecular dynamics (MD) and quantum mechanical simulations are to be utilized for uncovering the fundamental chemistry and physics of the system.
- Nudged Elastic Band method is employed to find the energy barriers between states during rotation.
- Density Functional Theory used to support MD results.

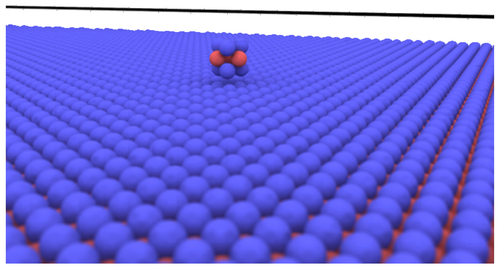
Frictional Properties: Energy Barrier to Rotation



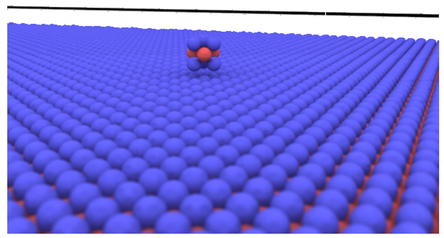
Starting structure of energy barrier



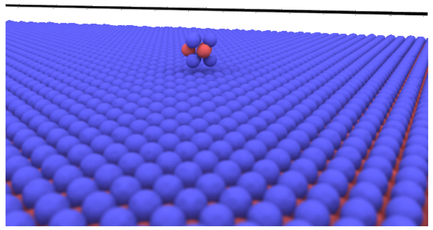
Energy barrier of unit cell rotating 60 degrees.



final structure of energy barrier after 60 degree rotation of unit cell



Visualization of unit cell rotation

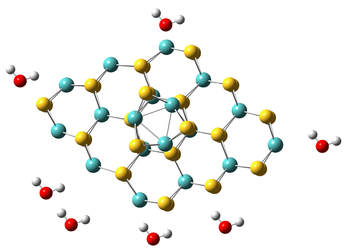


Visualization of unit cell rotation

MD simulation of unit cell rotating above slab.

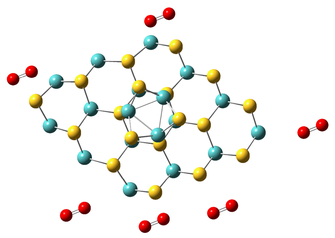
Influence of Local Surface Strain

The change in the electronic structure, due to strain, may facilitate the lowering of the energy barrier.



Model structure of water vapors around edge sites of MoS_2

Environmental molecules incorporated into the simulation to deduce their effect on frictional properties



Model structure of molecular oxygen around edge sites of MoS_2

Local strain used to investigate how local strain affects frictional properties and reactivity.

Future Work

- Gain a fundamental understanding of the relationships between frictional properties, reactivity, and strain.
- This knowledge could be used to develop more robust experimental setups

Acknowledgements

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