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Environmental Effects on the Tribological Properties of MoS_2

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We describe the adsorption of water and oxygen on MoS_2 and their effects on the tribological properties. Using a combination of density functional theory and molecular dynamics simulations we show that the presence of defects, notably sulfur vacancies, significantly increases the affinity of MoS_2 for adsorption of environmental species. Defect sites nucleate the formation of small clusters of molecules in the interlamellar space, strongly impacting the tribology of MoS_2. We will also present simulated isotherms for adsorption and oxygen at conditions representative of real-world applications of MoS_2.

Keywords: tribology, molybdenum disulfide, water adsorption, friction, humidity

Molybdenum disulfide (MoS_2) is a lamellar solid with many diverse applications including semiconductor devices, catalysis, and lubrication. The layers of MoS_2 interact via weak van der Waals forces, enabling the layers to slide with a coefficient of friction as low as $\mu \cong 0.01$ in dry or vacuum environments. The low friction coefficient makes MoS_2 an appealing solid lubricant for use in satellites and other aerospace applications where liquid lubricants are infeasible. However, exposure to environmental species, e.g. oxygen and water, has been shown to degrade the lubricating properties of MoS_2, limiting its usefulness for many potential applications. The precise mechanisms of these interactions and how they degrade tribological performance, however, remain poorly understood.

We report the results of density functional theory, Monte Carlo, and molecular dynamics simulations of the adsorption of water and oxygen on MoS_2 under realistic atmospheric conditions. We will discuss the interaction of water and oxygen with common defects in MoS_2, including sulfur vacancies and oxidized sites. We have computed adsorption isotherms adsorption for a range of realistic temperatures, humidity levels, and defect densities to determine the expected environment between MoS_2 layers and find that while pure MoS_2 is only slightly hydrophilic (contact angle $\geq 70^o$), the presence of defects greatly increases adsorption.[1] Defect sites, particularly S vacancies, are favorable adsorption sites and nucleate the formation of small clusters of molecules.

We also discuss how the presence of water and oxygen affect the structure of MoS_2 and its tribological properties.[2] Simulations show that intercalated molecules disrupt the crystal structure of MoS_2 and increase the energetic barriers to sliding, resulting in increased friction.

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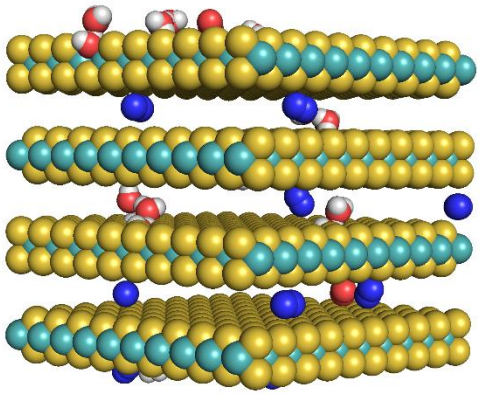

Figure 1: Screenshot of grand canonical Monte Carlo simulation of adsorption in MoS2 with defects at 313K and 50% RH. Atoms shown are Mo (cyan), S (yellow), O (red), N (blue) and H white).

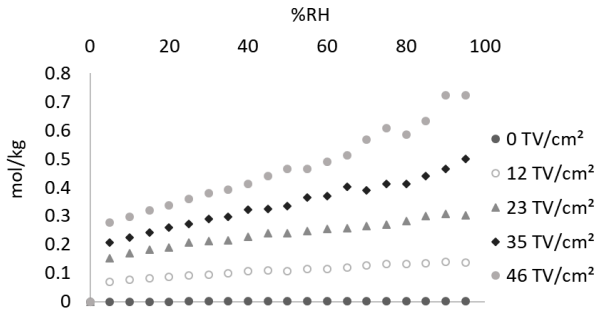

Figure 2: Adsorption isotherms for water in MoS_2 with various defect densities. (1 TV = 10^{12} vacancies)

References

1. N. S. Bobbitt and M. Chandross, Water adsorption in MoS2 under realistic atmospheric conditions, *in preparation*
2. Q. Moore, N.S. Bobbitt and M. Chandross, The effects of oxidation on friction in MoS_2, *in preparation.*