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# Effect of dissociated and physisorbed $H_2O$ on the friction of graphene and $MoS_2$

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The tribological behaviour of graphene and $MoS_2$ films depend on the environment. An increase in the relative humidity in the test atmosphere would reduce friction of graphene but increase that of $MoS_2$. Pin-on-disk tests, TEM, and first principles calculations showed that the dissociated $H_2O$ at sliding induced defects of graphene increased the layer spacing and reduced the interlayer binding energy ($E_B$) for a low coefficient of friction (COF). Meanwhile, the physisorbed $H_2O$ molecules at defect sites of $MoS_2$ formed hydrogen bonds with S, which increased $E_B$ and the COF by making the shearing between the $MoS_2$ layers more difficult.

**Keywords:** graphene, $MoS_2$, $H_2O$, friction, first principles calculations

## 1. Introduction

2D layered materials of graphene and $MoS_2$ can used to mitigate friction and adhesion between engineering surfaces when used as thin films and liquid lubricant additives. The low friction of graphene and $MoS_2$ has been generally attributed to the easy shear of the van der Waals force bonded layers. However, $H_2O$ molecules affect the frictional performances 2-D materials differently. Using experimental investigations and first principles calculations, we elucidate how dissociated and undissociated $H_2O$ molecules affect the interlayer binding energy and friction of graphene and $MoS_2$. The study also provided TEM evidence for the changes in interlayer spacings in the tribolayers.

## 2. Methods

### 2.1. Experimental details

Multilayer Graphene samples were deposited on Ni foils using a chemical vapour deposition (CVD) process. $MoS_2$ films were deposited on M2 steel disks using magnetron sputtering. The sliding counterfaces were Ti-6Al-4V. The sliding tests were conducted at a sliding speed of 0.05m/s under a normal load of 1N using a CSM tribometer in dry $N_2$ and in humid atmospheres (15%RH~82%RH). Raman and HR-TEM were used to identify the defect structures of graphene and $MoS_2$ before and after sliding tests.

### 2.2. First principles calculations

The calculations were conducted using PAW-PBE potential within the frame of vdW-DF2 in VASP package. A monovacancy in (6×6) graphene cell and a triple vacancy in (4×4) $MoS_2$ cell with 15 Å vacuum layer were used to estimate the how $H_2O$ molecules physi- and chemisorbed at defect sites of graphene and $MoS_2$. Grids of 4×4×1 and 5×5×1 k-points were used for graphene and $MoS_2$ slabs respectively. The plane-wave cut off energy was 500 eV. The electronic degree of freedom and the Hellman-Feynman forces were converged to $10^{-5}$ eV/cell and 0.05 eV/Å.

### 2.3. Results

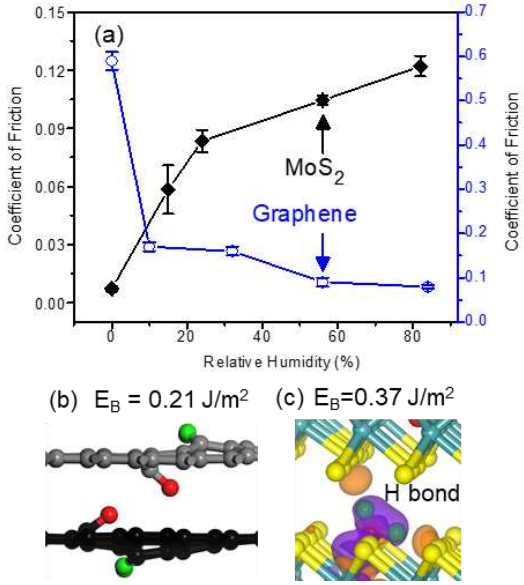


Figure 1: (a) COF of graphene and $MoS_2$ as a function of relative humidity; (b) Dissociated $H_2O$ reduced $E_B$ of graphene; (c) Undissociated $H_2O$ forms H···S bond and increases $E_B$ of $MoS_2$. (Atoms: black and grey for C, red for O, green for H, yellow for S, cyan for Mo.)

## 3. Discussion

Although graphene was initially defect free, sliding induced defects would form and dissociate $H_2O$, and the dissociated H and O would passivate the dangling bonds and reduce the $E_B$, which agreed with TEM observations increased layer spacing of graphene in the transfer layers, and consequently the COF was reduced. On the other hand, $H_2O$ could also dissociate at defect sites of $MoS_2$, such as a triple vacancy, a process that may contribute to formation of $MoO_3$. But the dissociated $H_2O$ was not effective in increasing the $E_B$. The undissociated $H_2O$ would form H bonds with S on $MoS_2$, a process that increased the $E_B$ TEM of the parallel reoriented $MoS_2$ layers at the transfer layers with reduced layer spacings would lead to an increase in the interfacial strength and thus a COF was expected (Fig.1). The investigation provides new insight on designing new types of coatings that are suitable for harsh environments.