

Force Field Development for Exfoliation of MoS₂

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Materials Genome Innovation
for Computational Software



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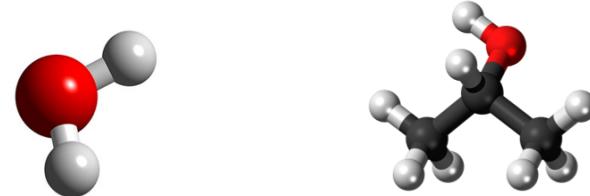
Force Fields

Compounds in the system:

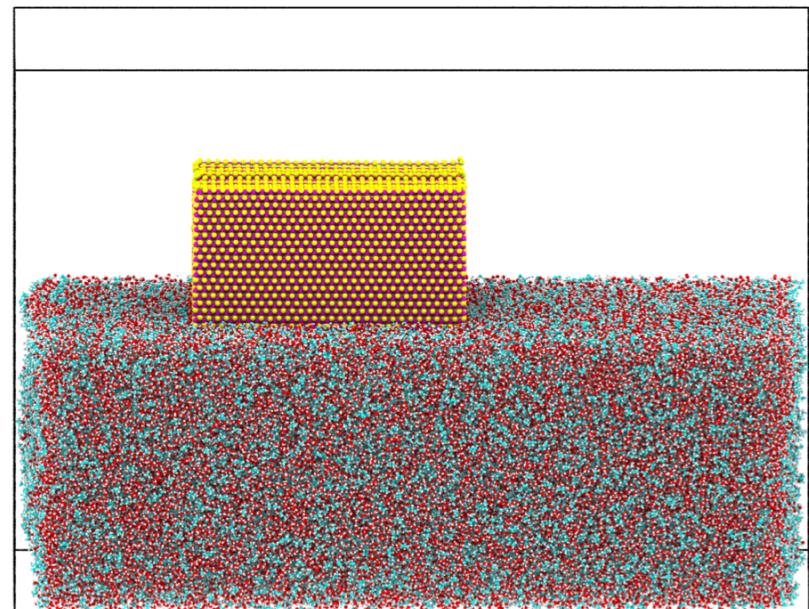
- Water
- isopropyl alcohol(IPA)
- MoS_2

We need force fields:

- For each compounds
- Between Water, IPA,
 MoS_2



Exfoliation Simulation Setup



Functional forms of Force Fields

- MoS₂ Reactive Empirical Bond Order REBO

$$E_b = \frac{1}{2} \sum_{i \neq j} f_{ij}^C(r_{ij}) [V^R(r_{ij}) - b_{ij} V^A(r_{ij})]$$
$$= \frac{1}{2} \sum_{i \neq j} f_{ij}^C(r_{ij}) \left[\left(1 + \frac{Q}{r_{ij}} \right) A \cdot e^{-\alpha \cdot r_{ij}} - b_{ij} B \cdot e^{-\beta \cdot r_{ij}} \right].$$

- Water TIP4P/2005

$$E = E_{bond} + E_{angle} + E_{coulomb} + E_{vdW}$$

- Isopropyl OPLS-AA

$$E = E_{bonds} + E_{angles} + E_{dihedrals} + E_{nonbonded}$$

- Lennard Jones Interaction Between MoS₂, water, and IPA

$$E_{LJ} = 4\epsilon \left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^6}{r^6} \right)$$

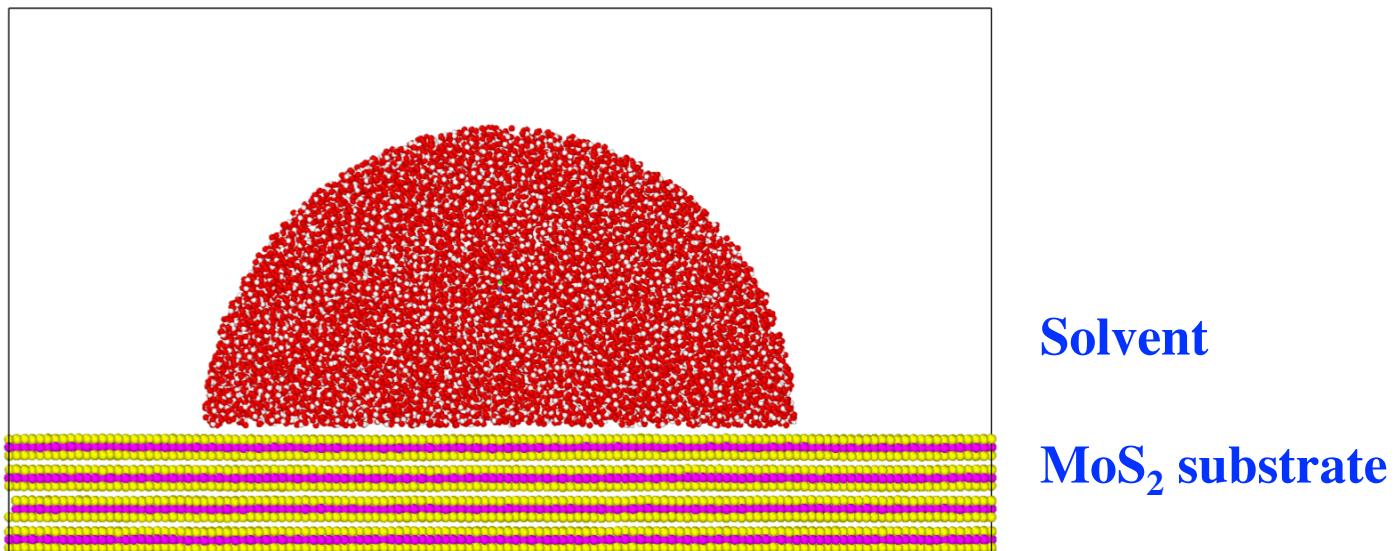
$$\epsilon_{ij} = \sqrt{\epsilon_i * \epsilon_j}, \sigma_{ij} = \sqrt{\sigma_i * \sigma_j}$$



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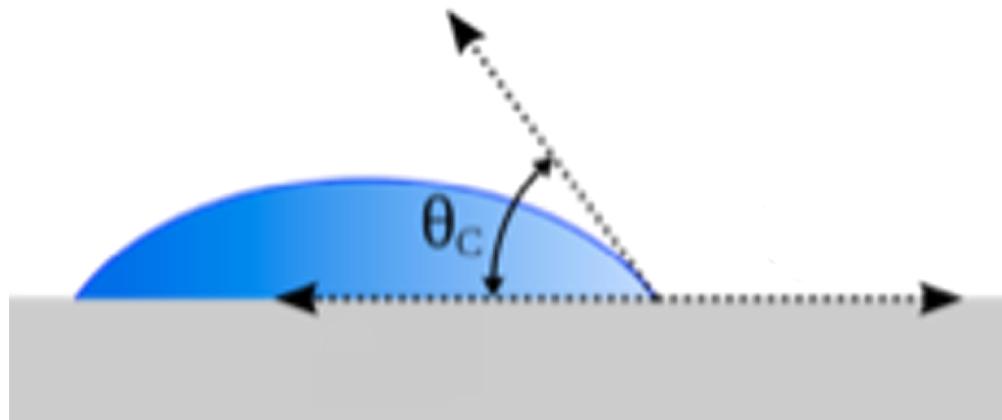
Simulation Procedure for Force Field Validation

- 1) Create and relax the liquid and MoS₂ separately
- 2) Hands-on: Place liquid droplet on MoS₂ and relax the system at 25°C in NVT ensemble



Force Field Validation

Hands-on: Measure the contact angle



Force field is tuned to match the experimental value of contact angle.

$$E_{LJ} = 4\epsilon \left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^6}{r^6} \right)$$
$$\epsilon_{ij} = \sqrt{\epsilon_i \times \epsilon_j}$$

Hands-on Directory

./wca/

|— lmp_mpi*

..... lammps executable file

|— ffield.ff

..... force field file

|— MoS.REBO.real.set5b

..... REBO force field for MoS₂

|— in.sys

..... input script to combine mixture and MoS₂

|— in.continue

..... input script for continue running

|— job1.pbs

..... pbs script to submit job for in.sys

|— job2.pbs

..... pbs script to submit job for in.continue

|— data/

..... output data

|— restart/

..... state data file

|— MoS2/

..... create MoS₂ substrate

|— water/

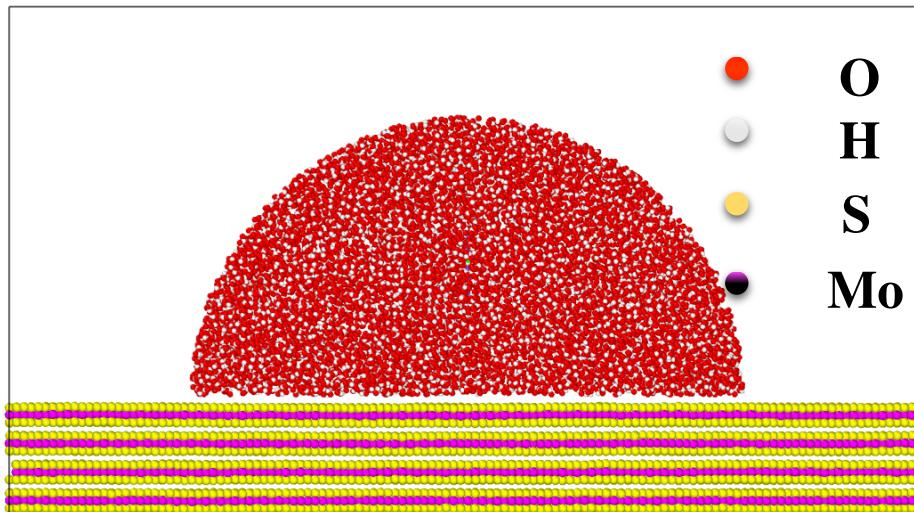
..... create liquid droplet



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Hands-on Step 1: Combine and Relax mixture and MoS₂

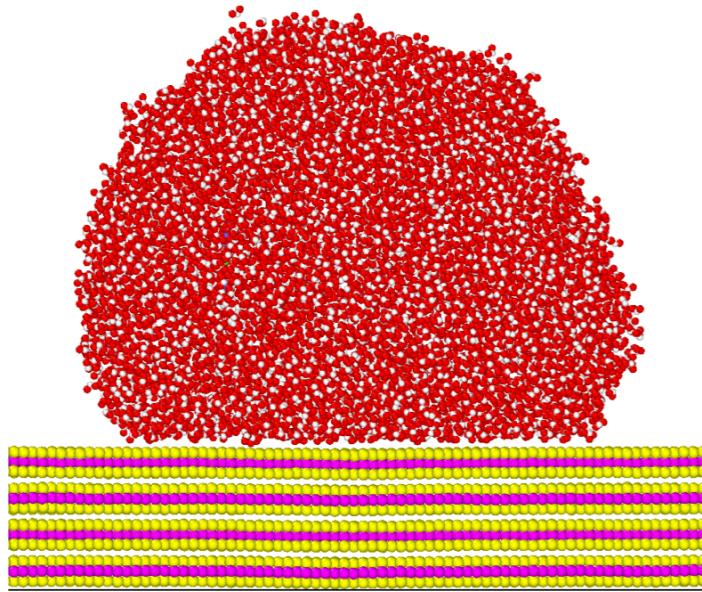
```
region·mybox·block·0.0·10.0·0.0·10.0·0.0·110.0·units·box·
create_box·4·mybox·bond/types·1·angle/types·1·&·
.....extra/bond/per/atom·2·extra/angle/per/atom·1·
read_data···./MoS2/data.MoS2·add·append·offset·2·1·1·1·1·
read_data···./water/data.water·add·append·shift·0.0·0.0·26.0|
```



File: ./wca/in.sys

Hands-on Step 1: Combine and Relax mixture and MoS₂

```
velocity·wat·zero·linear···  
velocity·MoS2·zero·linear···  
fix·mom·MoS2·momentum·10·linear·0·0·1···  
···  
fix·nvt·all·nvt·temp·300.0·300.0·100.0|
```



File: ./wca/in.sys



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Hands-on Step 1: Submit the Job

Copy the file to your directory:

cp -r .. /magics35/wca .

Submit job:

cd ./wca

qsub job2.pbs

Monitor job:

qstat -u your-user-name

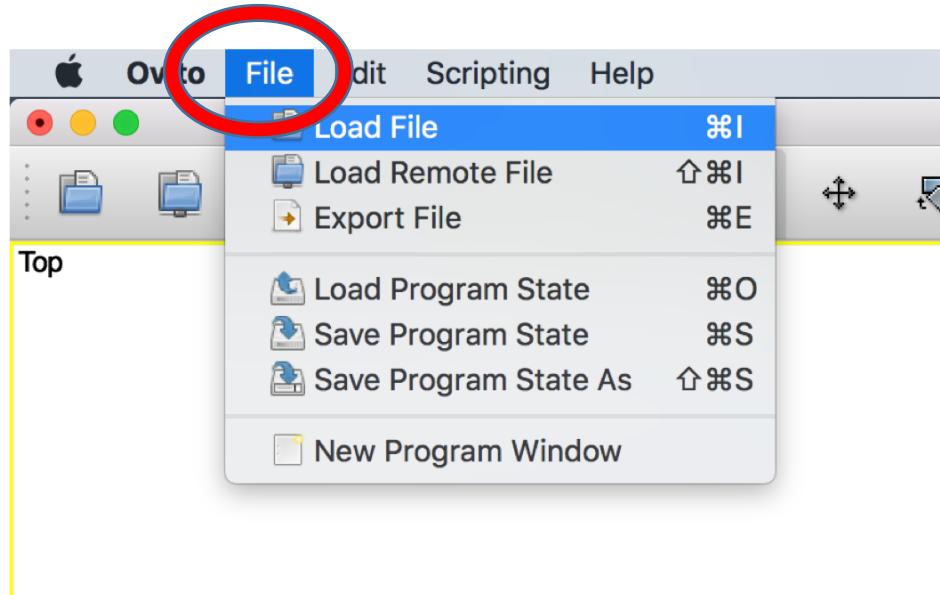


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Hands-on Step 2: Measure the Contact Angle

- Download the trajectory data into your laptop
 - `scp -r magicsXX@hpc-login3.usc.edu:/staging/magics18/magicsXX/wca/data .`
- Load the trajectory data into ovito

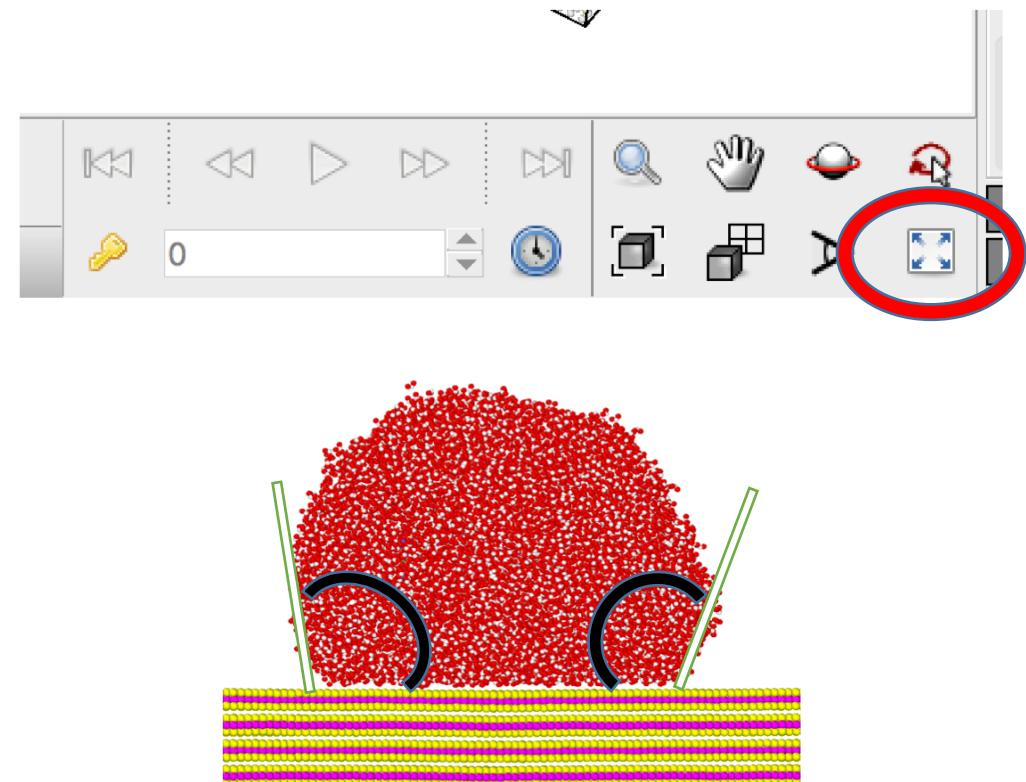
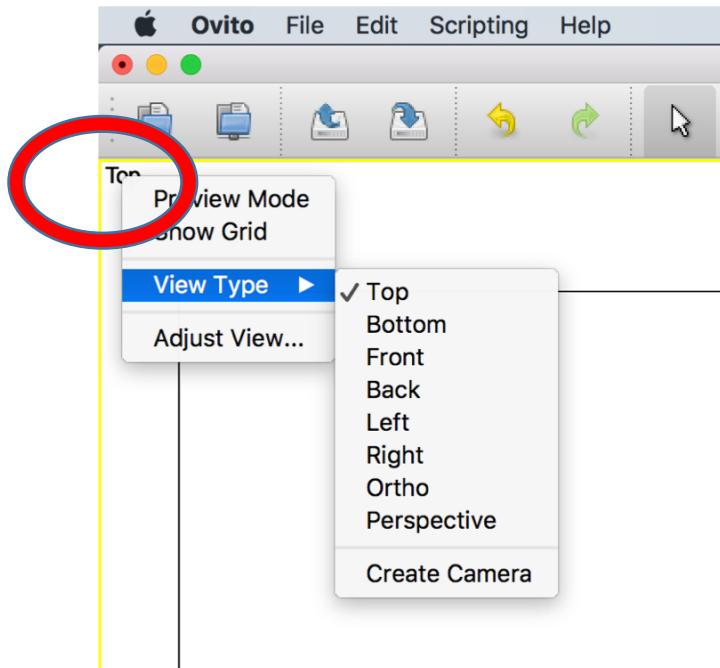


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Hands-on Step 2: Measure the Contact Angle

- Choose View Type ->Top
- Enter Full Screen mode



Force Field Validation

Contact Angle of Water/IPA mixture on MoS₂

