is paper describes objective technical results and analysis. Any subjective views or opinions that might be expres
the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Governm

SAND2019-10335C

MoS_2 in the Real World: Extending an Ideal Model to Water, Oxygen, and Defects

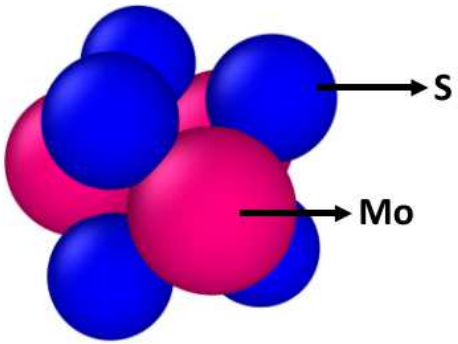
Adam R. Hinkle, John Curry, Nicolas Argibay, Michael T. Dugger, and Michael Chandross

Sandia National Laboratories, Albuquerque, NM, USA

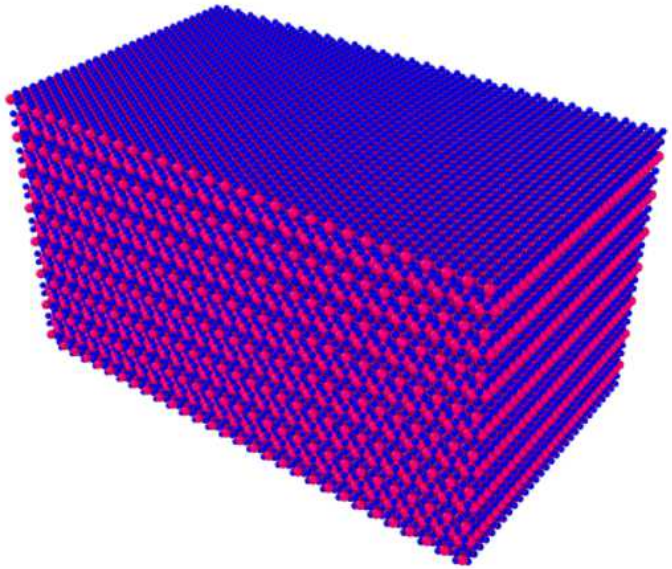
ACS 2019, San Diego

oratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, neywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract

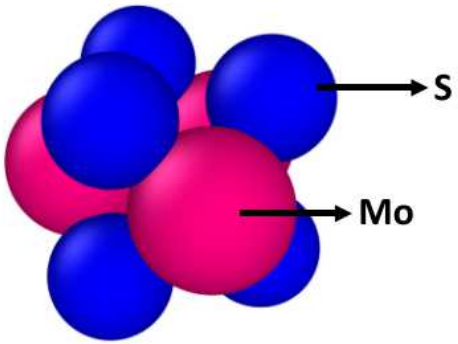
Motivation & Background



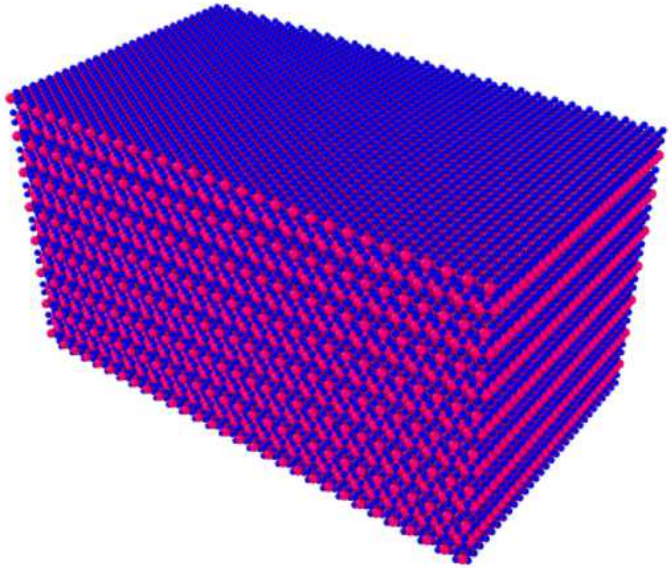
Molybdenum disulfide (MoS_2)



Motivation & Background



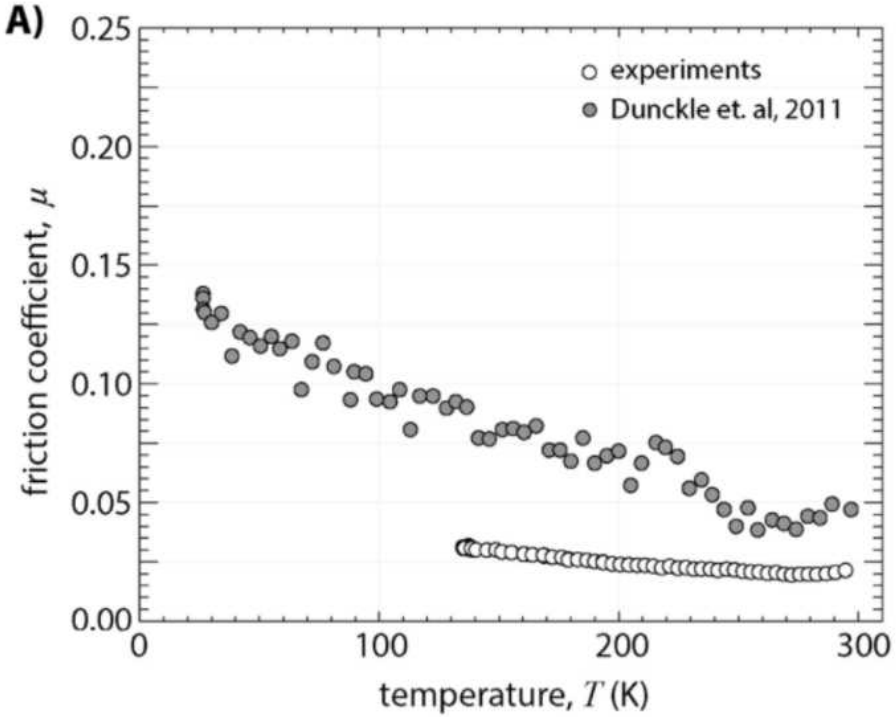
Molybdenum disulfide (MoS_2)

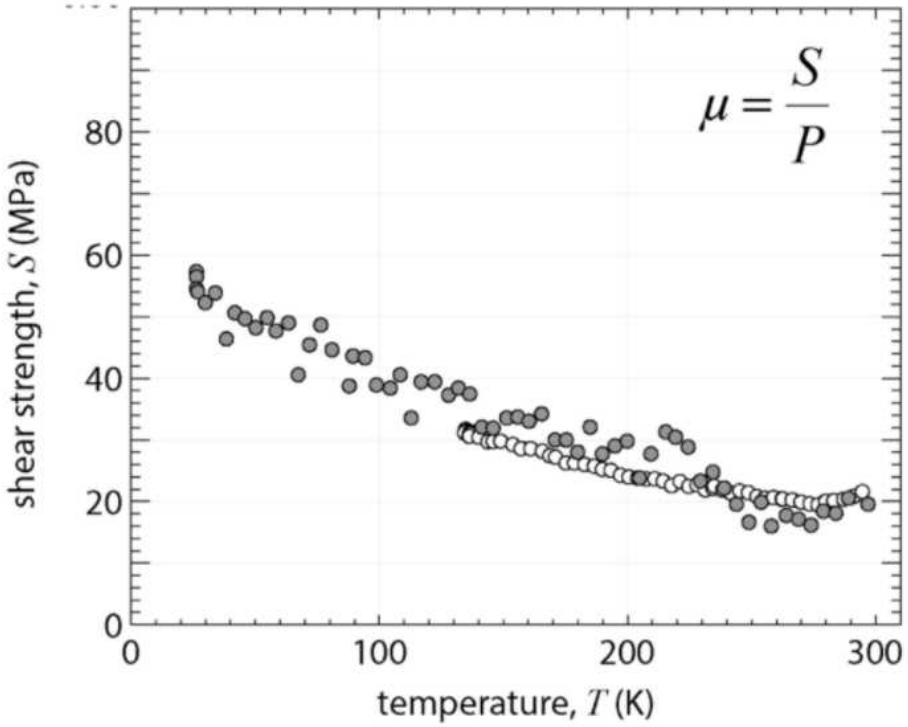


Space:

- operate in vacuum (+atomic oxygen in low earth orbit)
- store months – years before use; generally non-serviceable
- operating temperatures from 50 – 300K, depending on location
- large investments of time and money
- many mechanisms operate in run-in regime dominated by aging mechanisms

T-dependence $\mu = \mu(T, P)$ and $S = S(T)$ via MoS_2 Friction Experiments



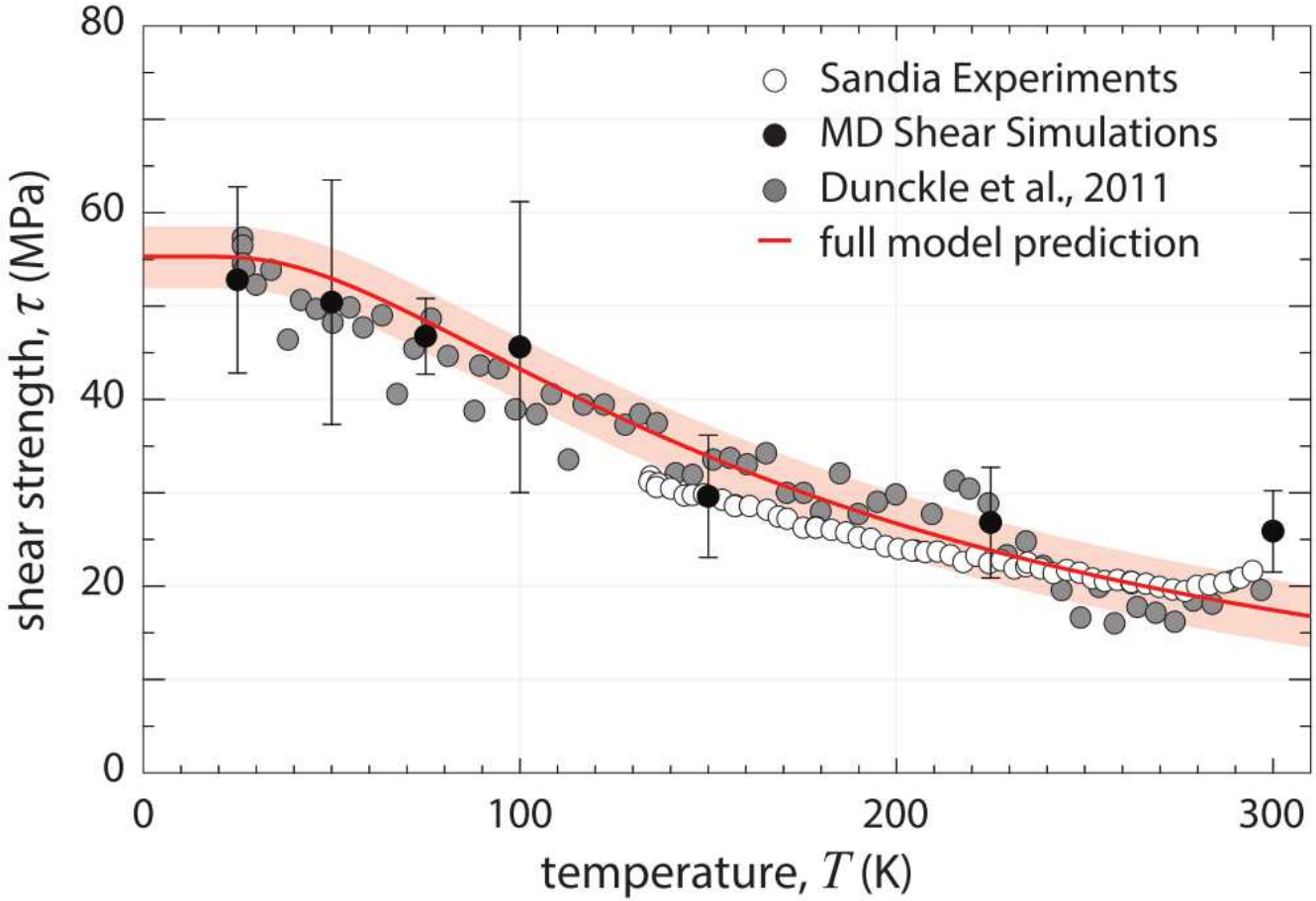


Curry and Hinkle, et al., ACS Appl. Nano Mater. (2018) 1, 10

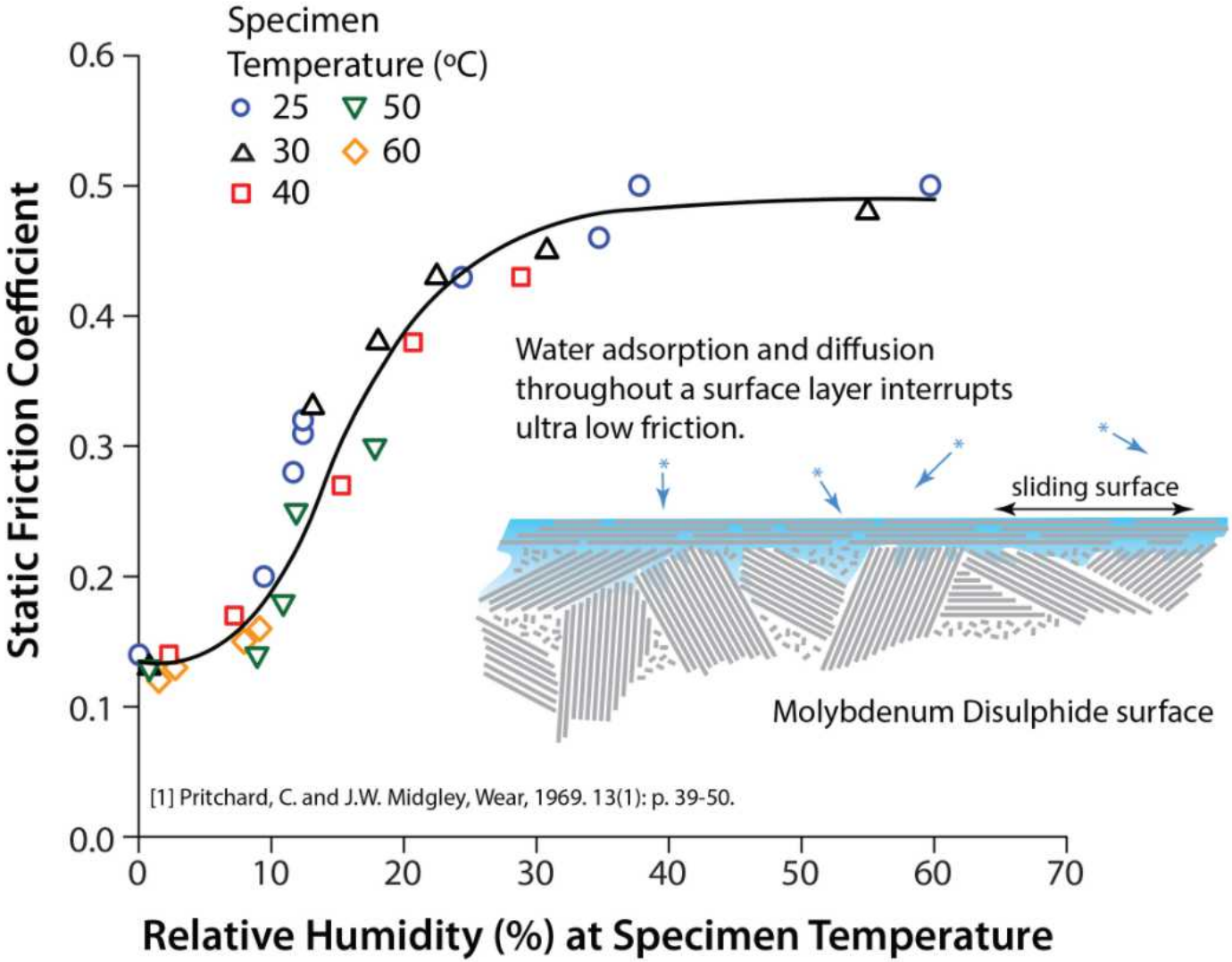
$$S(T) = S_L \left(1 - \exp\left(-\frac{\Delta E_i + \Delta E_r}{k_B T}\right) - \exp\left(-\frac{\Delta E_c}{k_B T}\right) + \exp\left(-\frac{\Delta E_r + \Delta E_c}{k_B T}\right)\right)$$

Curry and Hinkle, et al., ACS Appl. Nano Mater. (2018) 1, 10

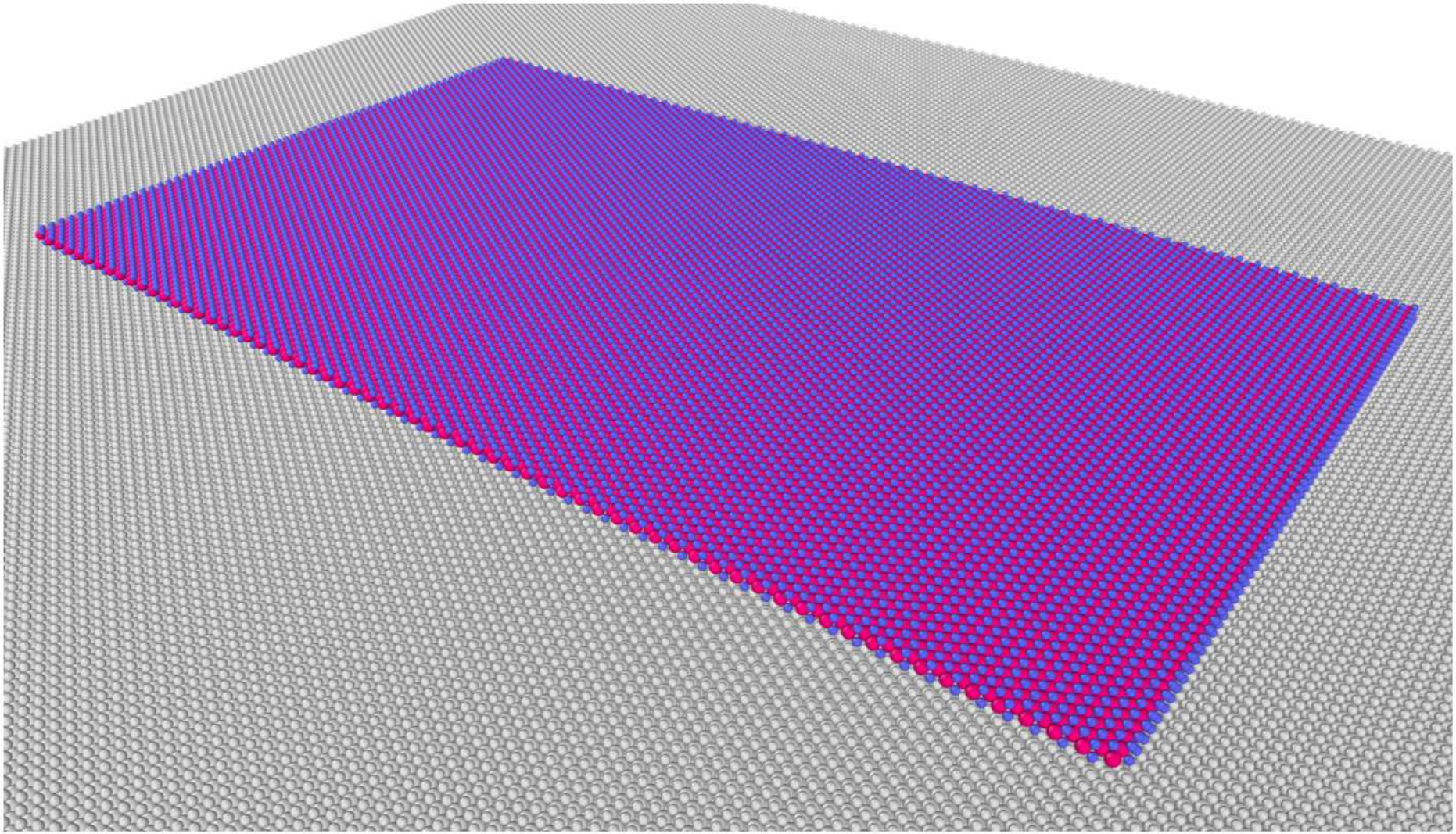
$$S(T) = S_L \left(1 - \exp\left(-\frac{\Delta E_i + \Delta E_r}{k_B T}\right) - \exp\left(-\frac{\Delta E_c}{k_B T}\right) + \exp\left(-\frac{\Delta E_r + \Delta E_c}{k_B T}\right)\right)$$



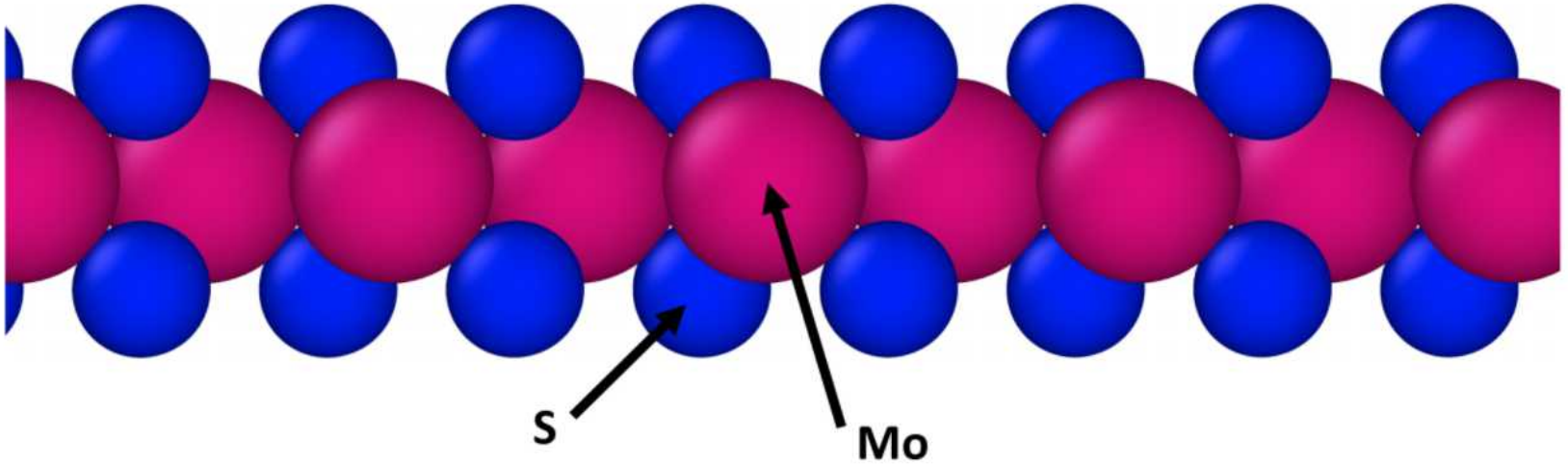
Effect of Water on Friction of MoS_2



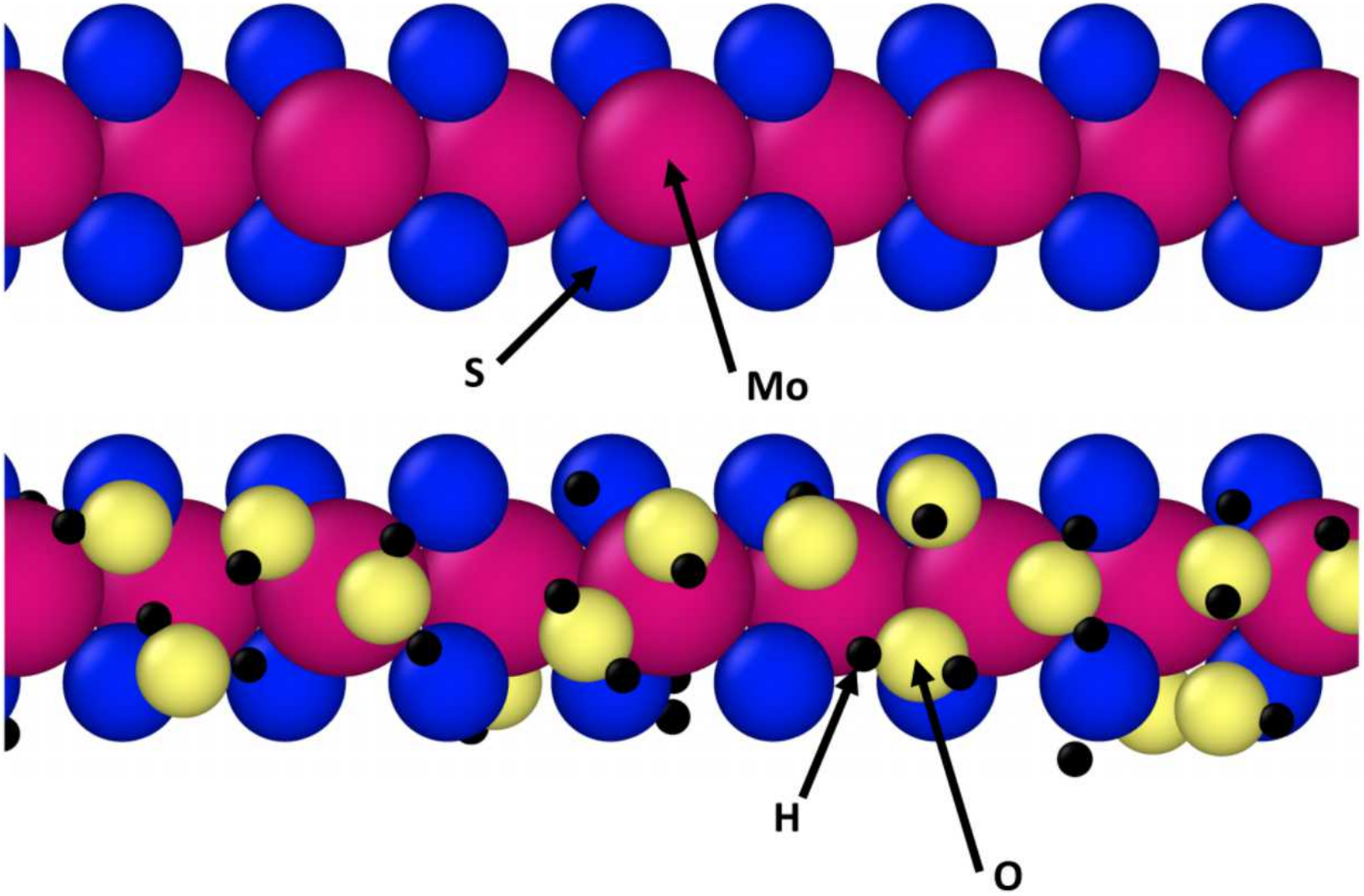
Effect of Water on Friction of MoS_2; 700nm^2 Flakes



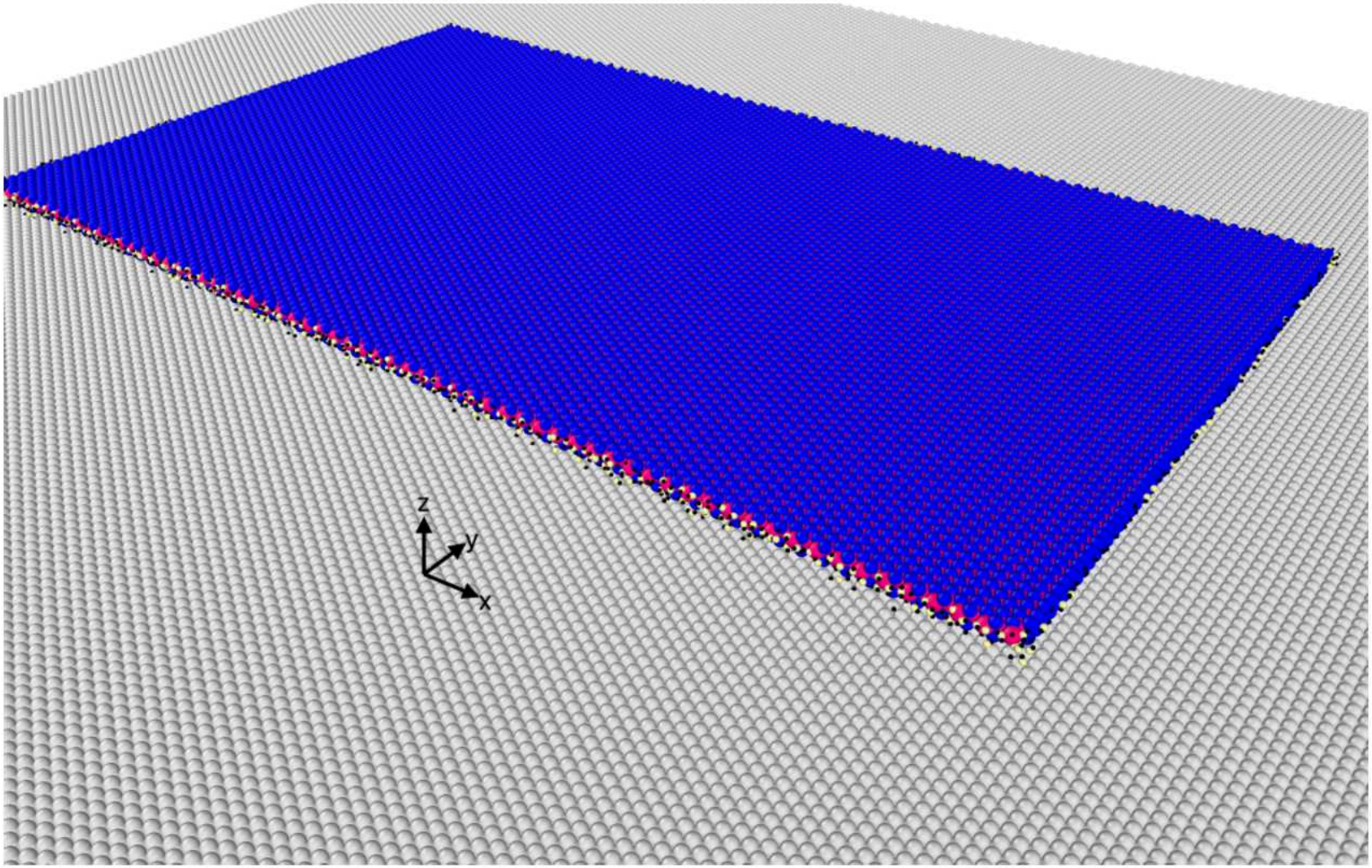
Effect of Water on Friction of MoS_2



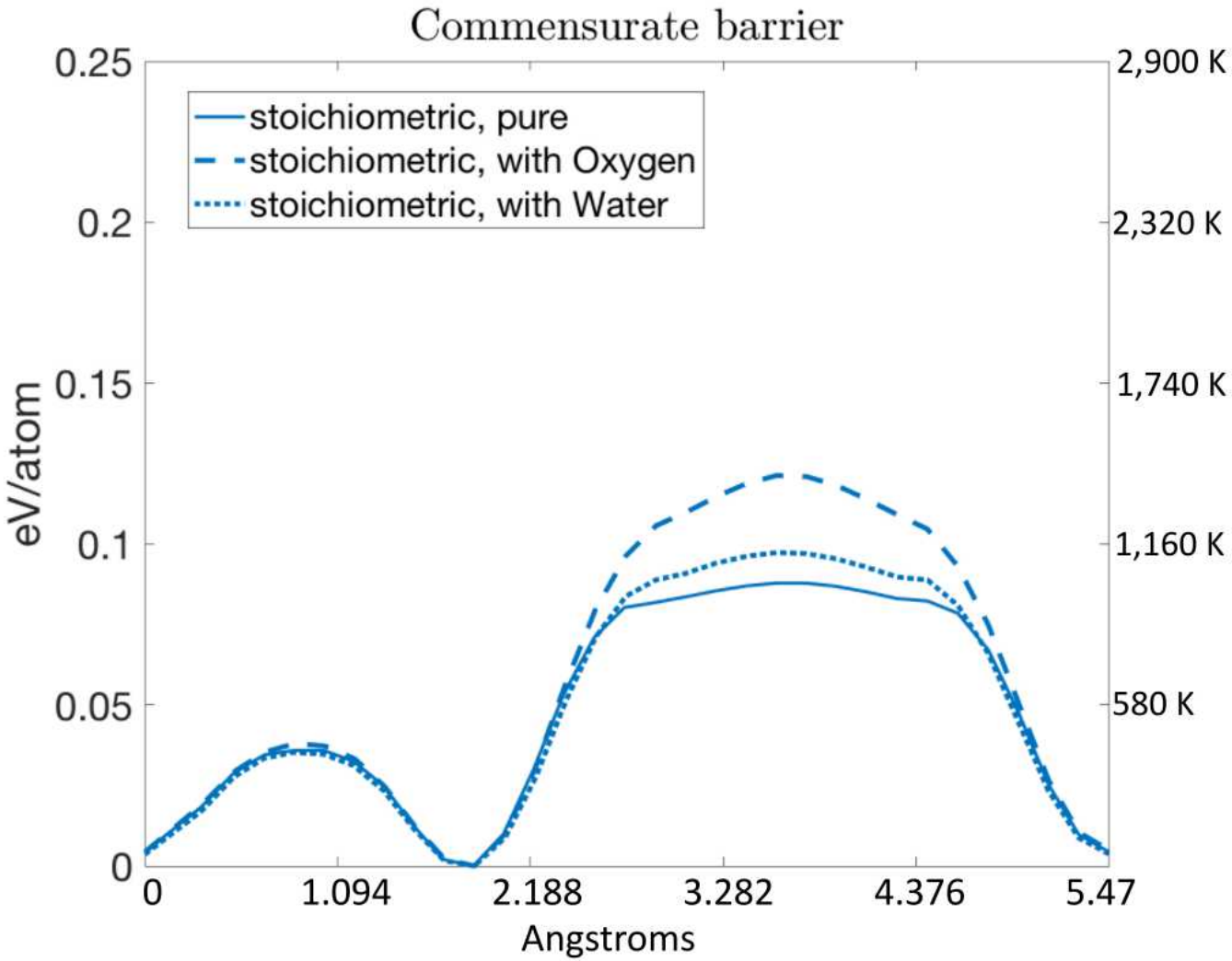
Effect of Water on Friction of MoS_2



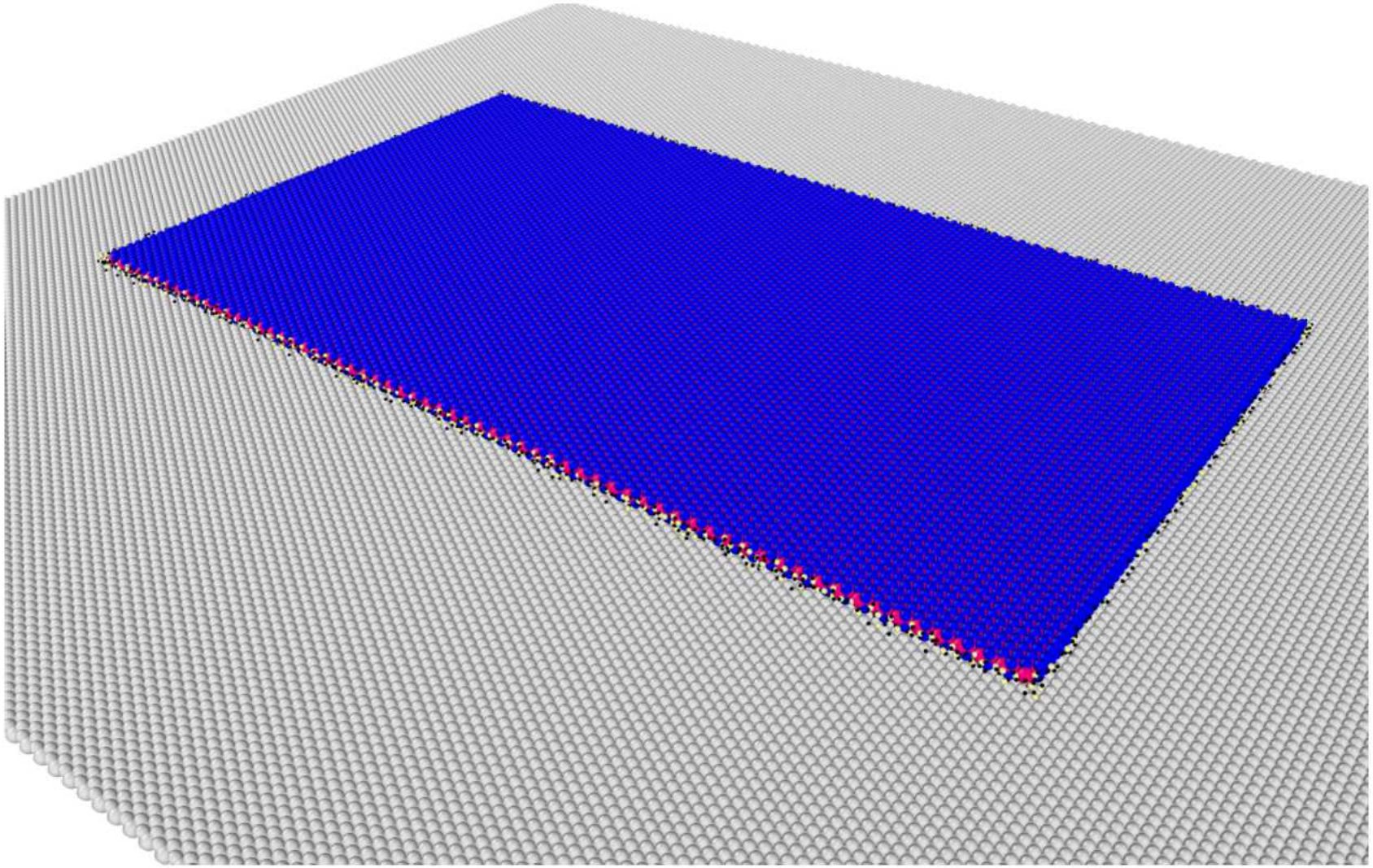
NEB Commensurate Sliding with H_2O and O_2



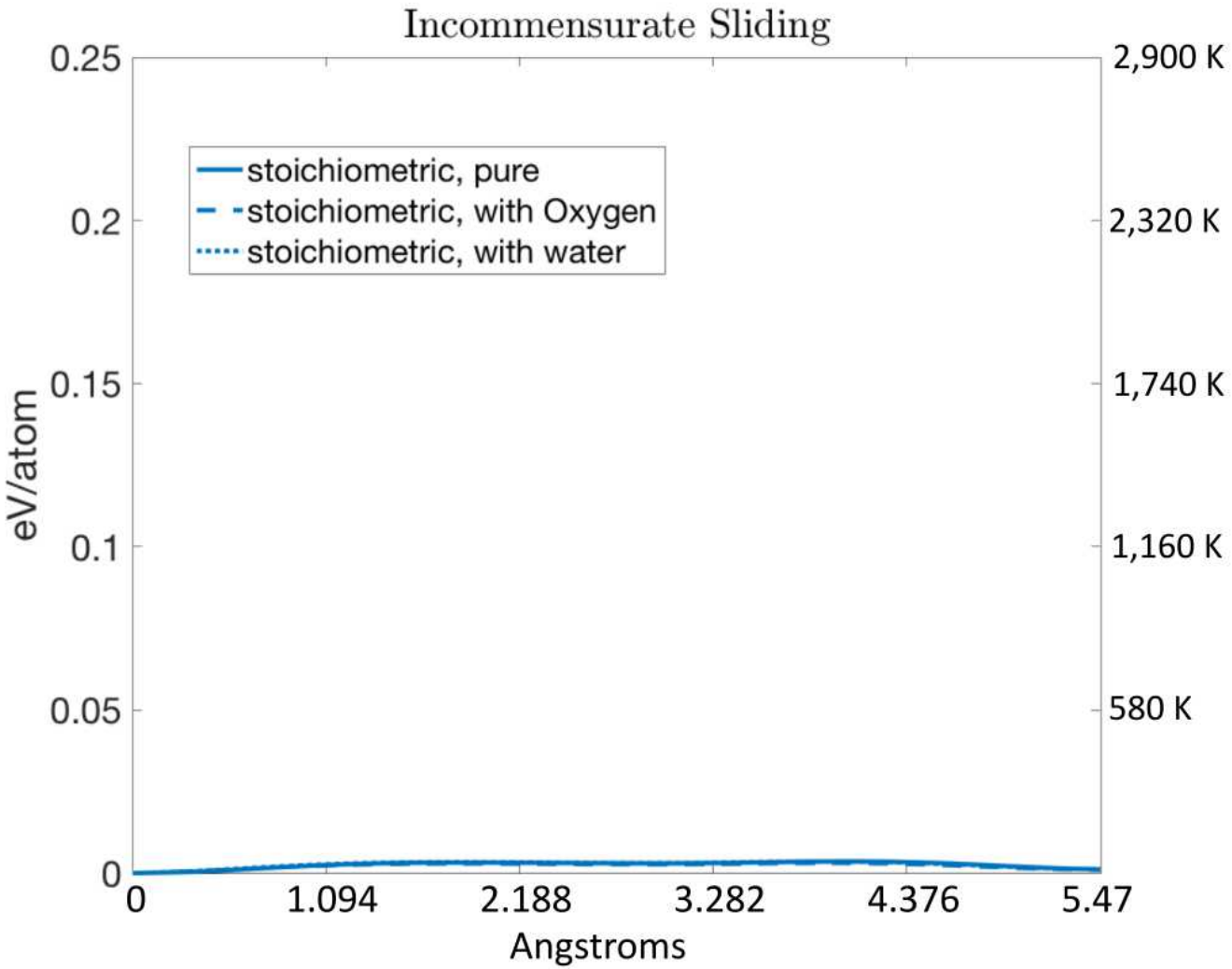
Effect of Water on Friction of MoS_2



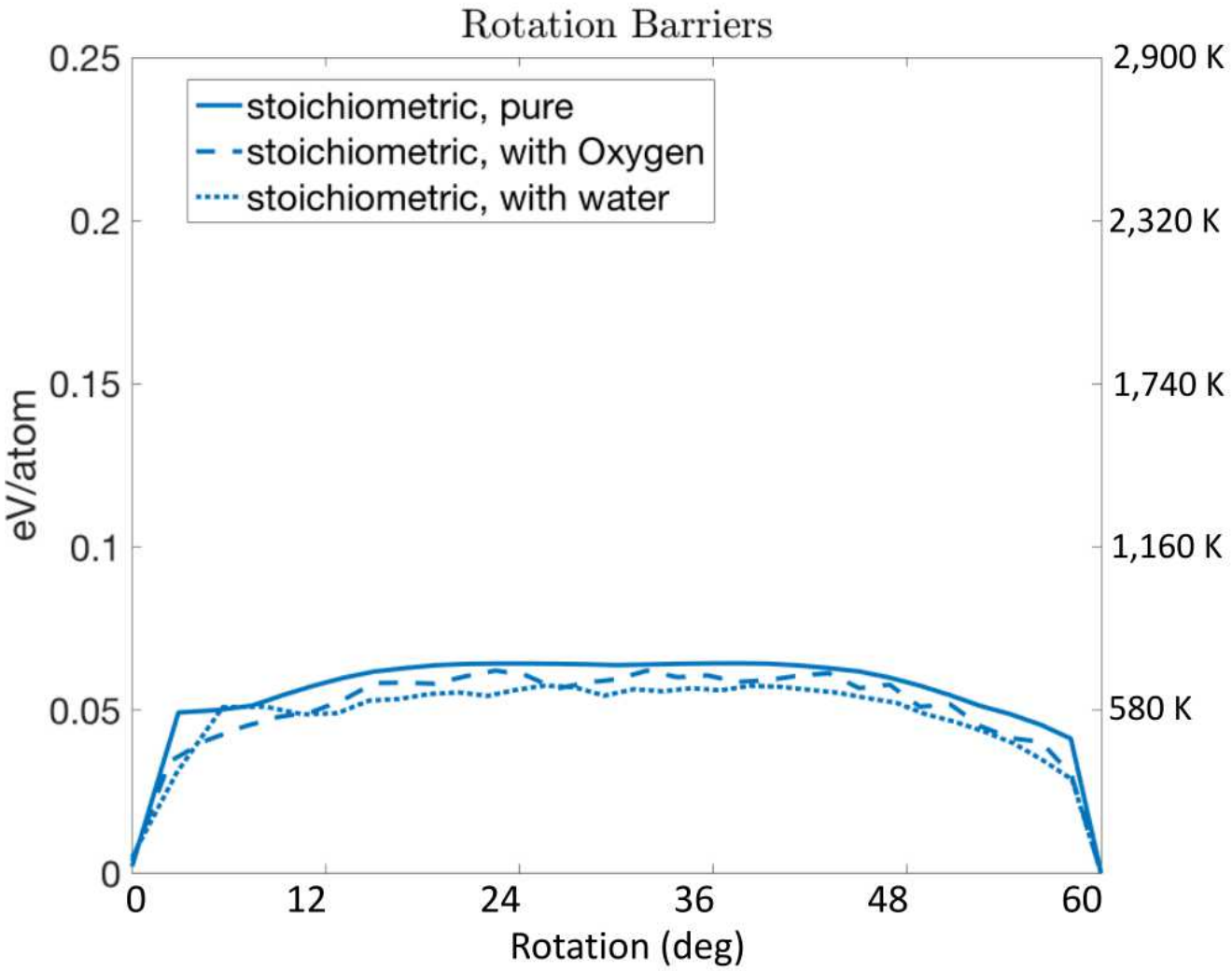
NEB Flake Rotation and Incommensurate Slide with H_2O and O_2



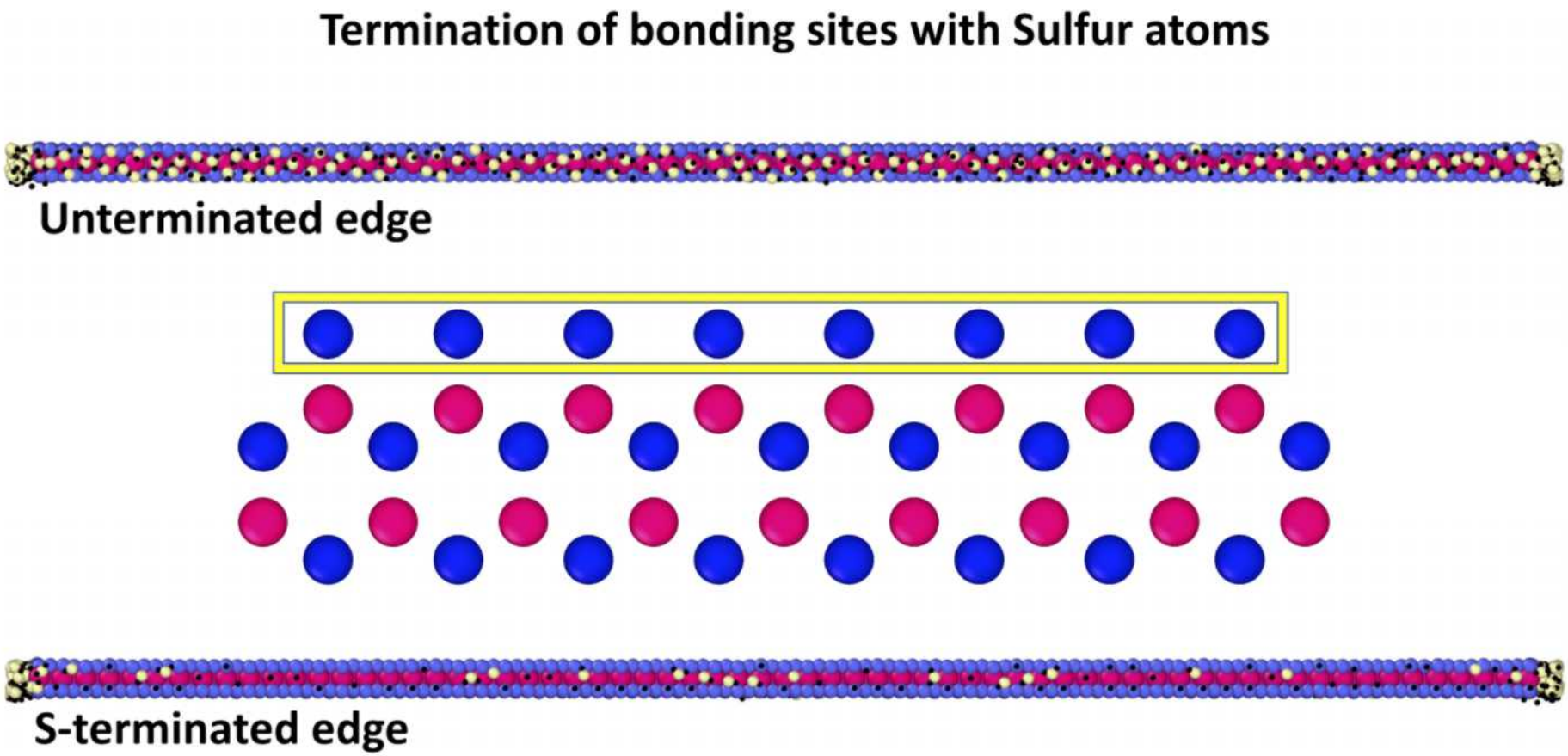
Effect of Water on Friction of MoS_2



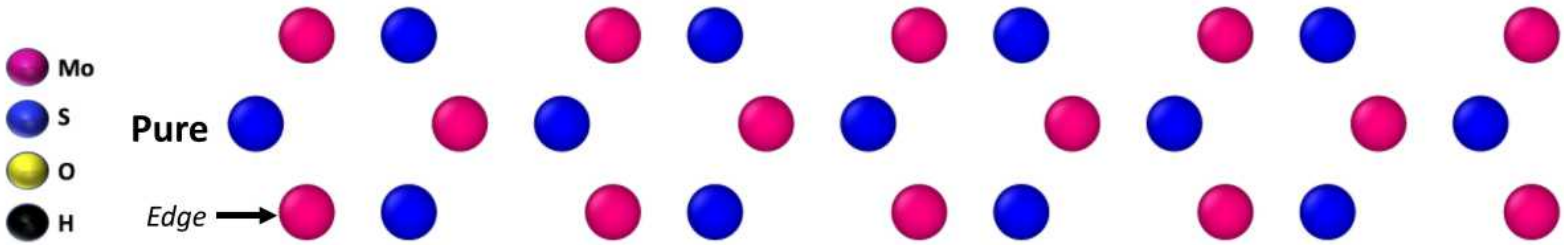
Effect of Water on Friction of MoS_2



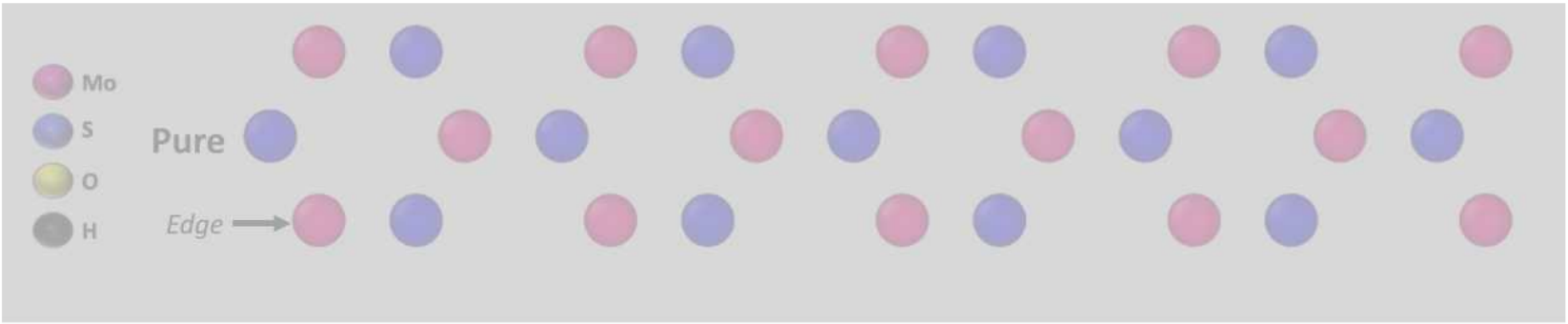
Effect of Water on Friction of MoS_2

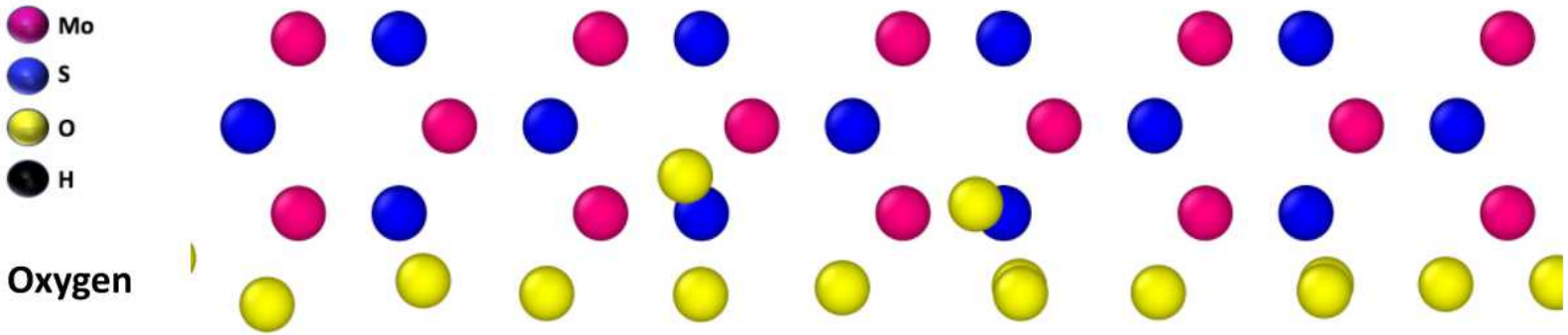


Defects: Exposed Mo

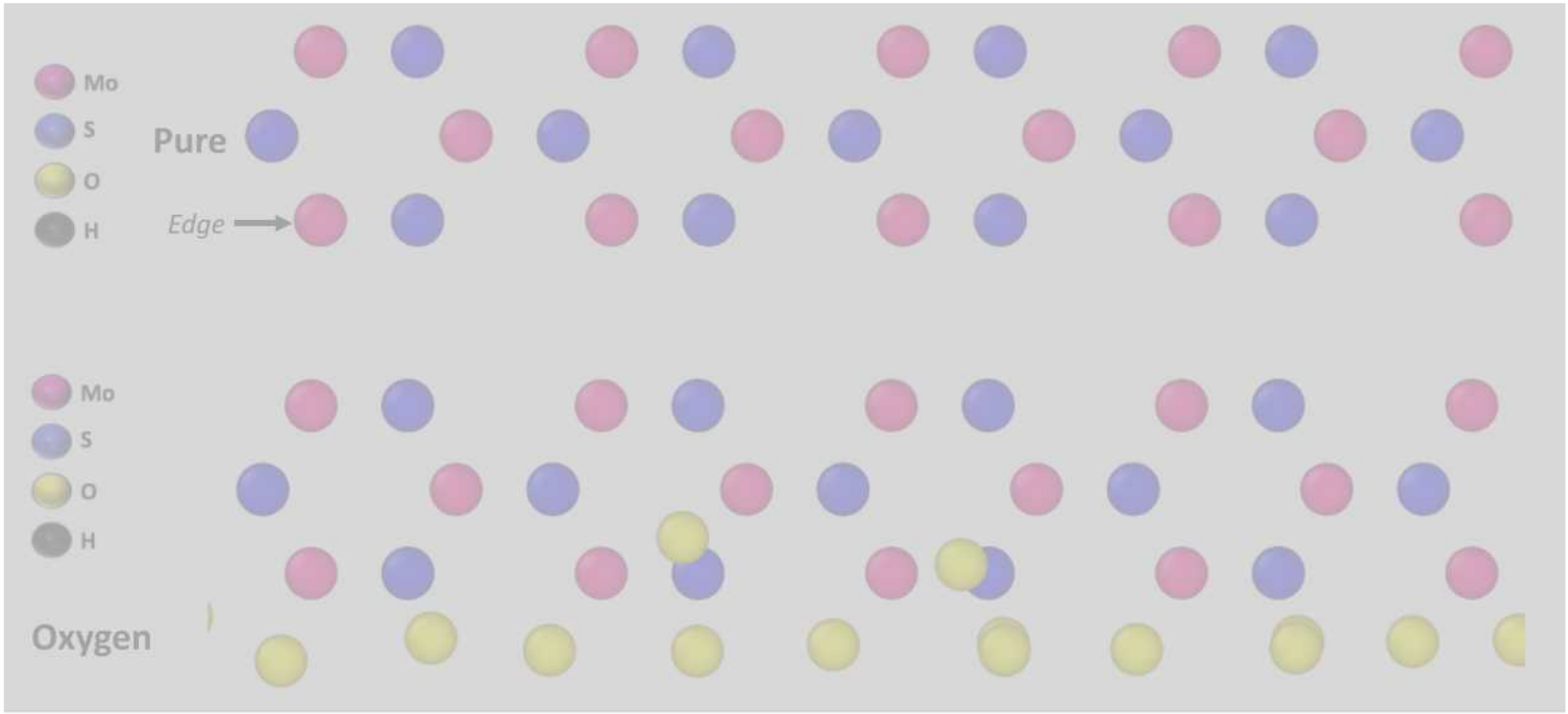


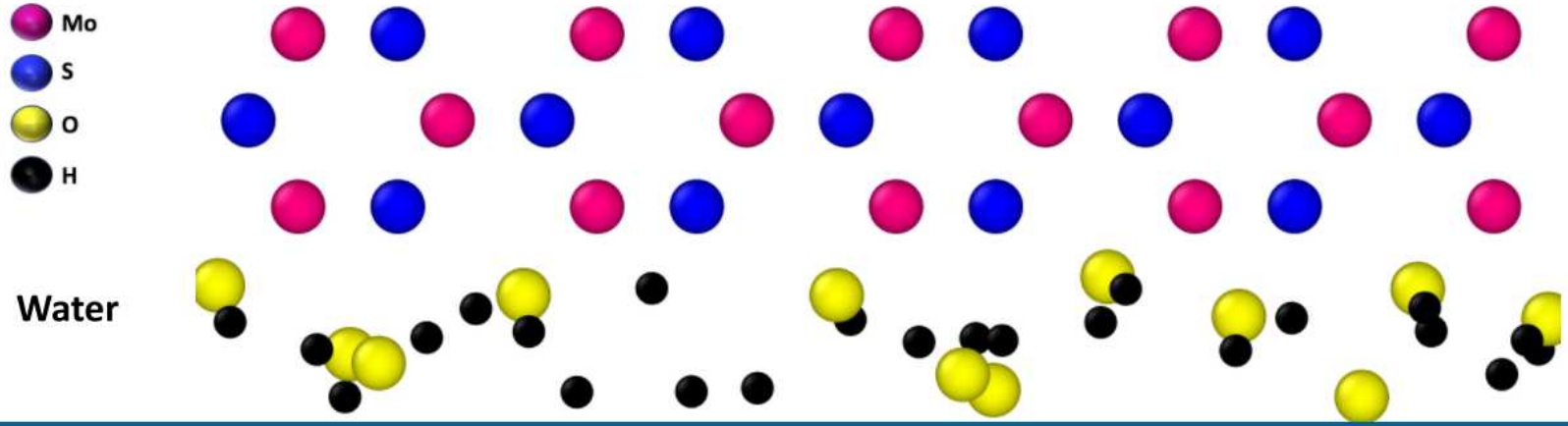
Defects: Exposed Mo with Oxygen



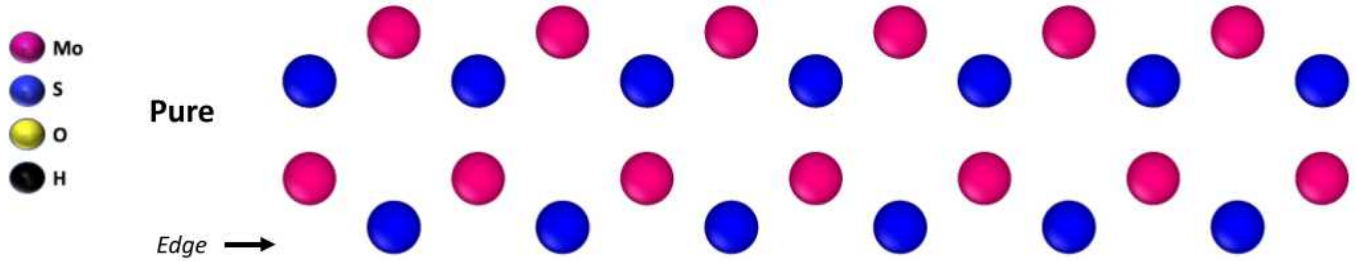


Defects: Exposed Mo with H_2O

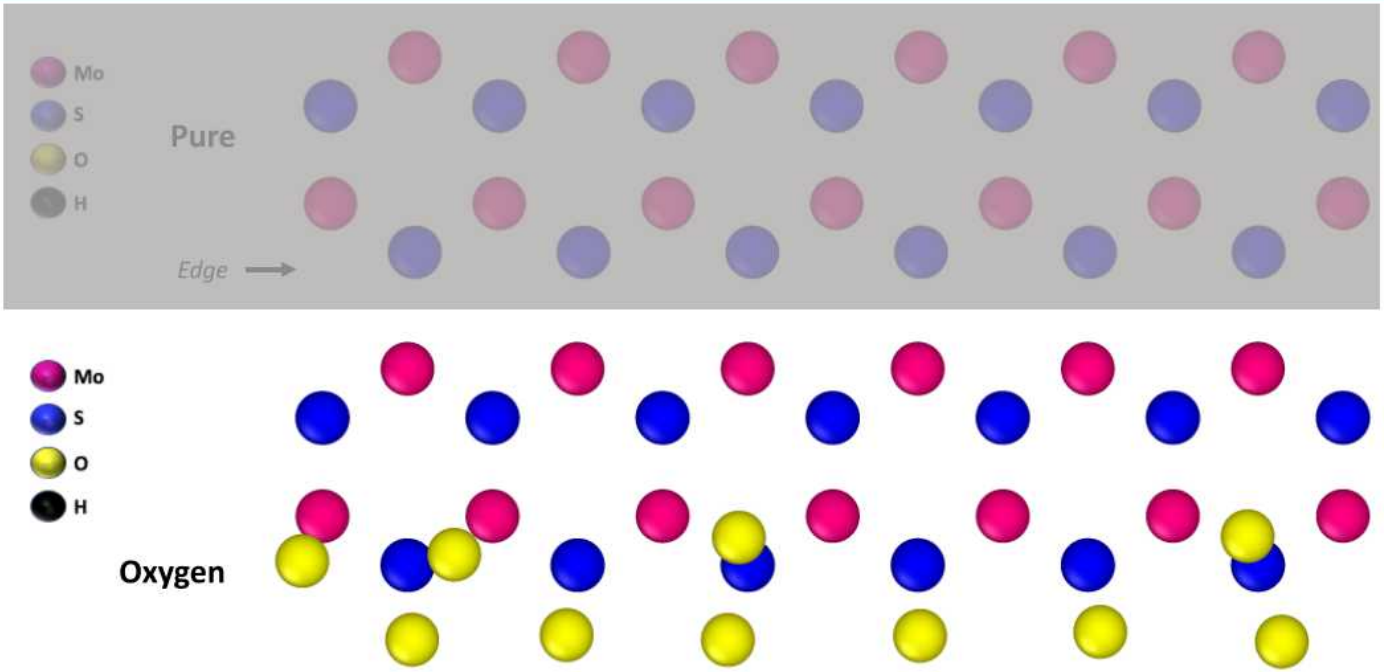




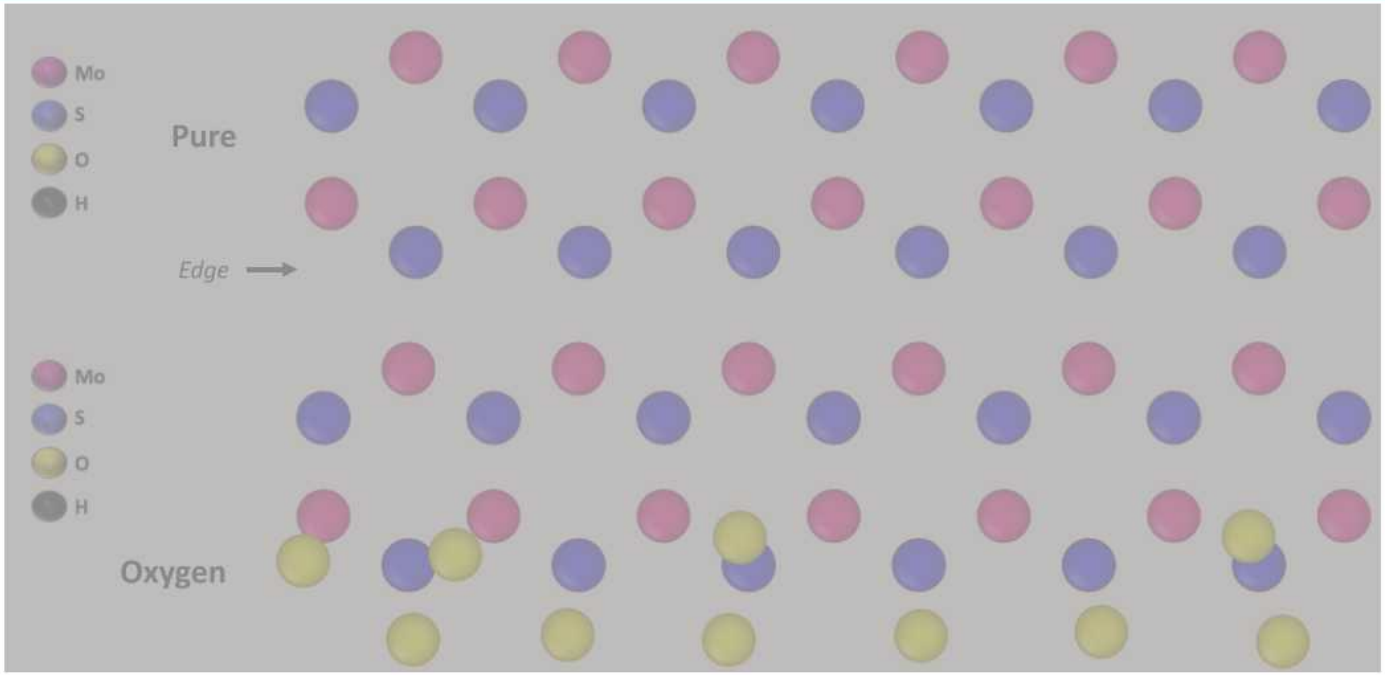
Defects: Exposed S

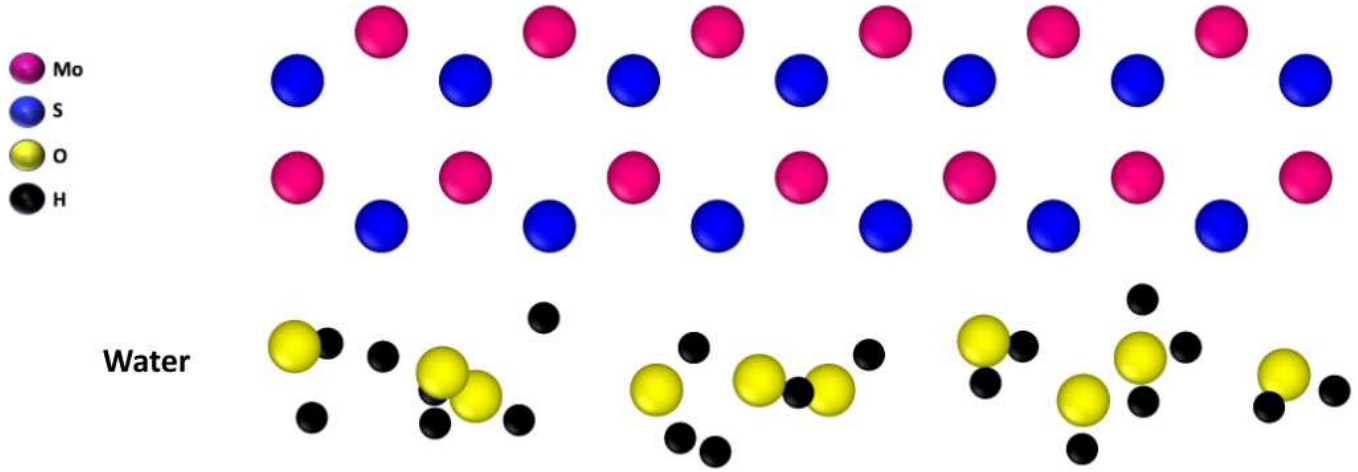


Defects: Exposed S with Oxygen

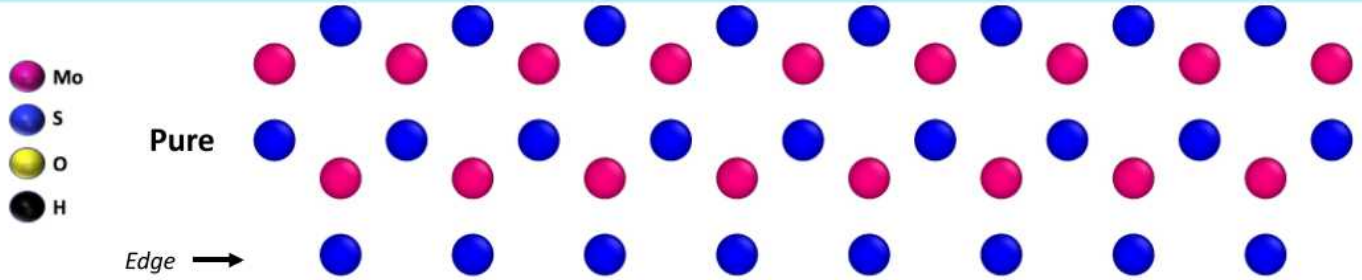


Defects: Exposed S with H_2O

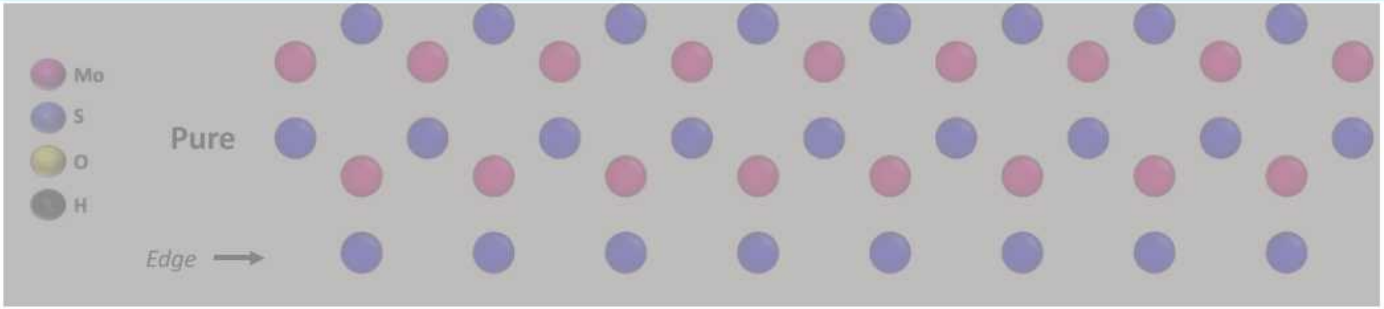


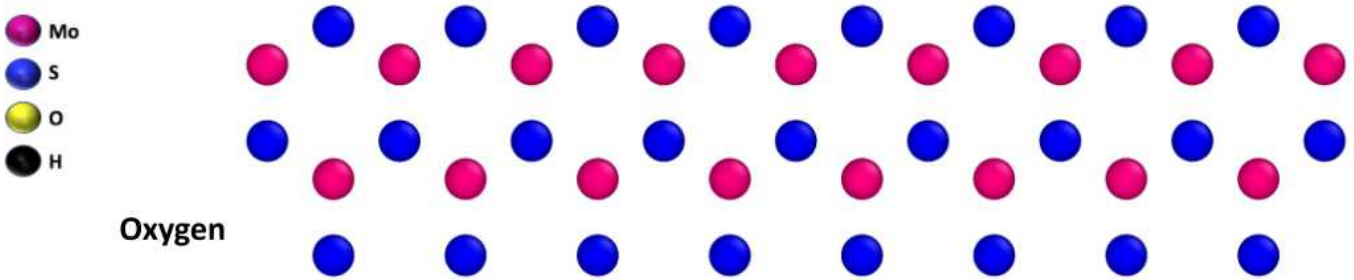


Defects: Added S (66.8% S, 33.2% Mo)

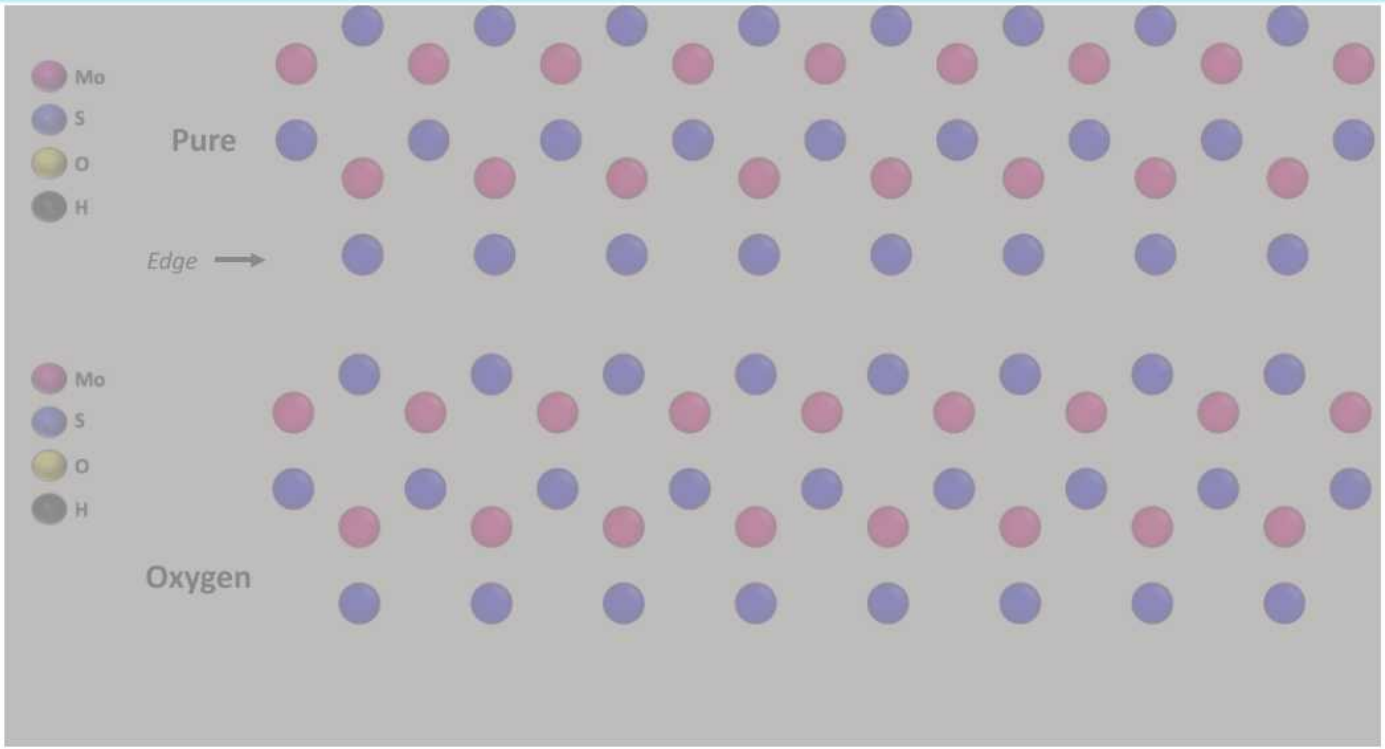


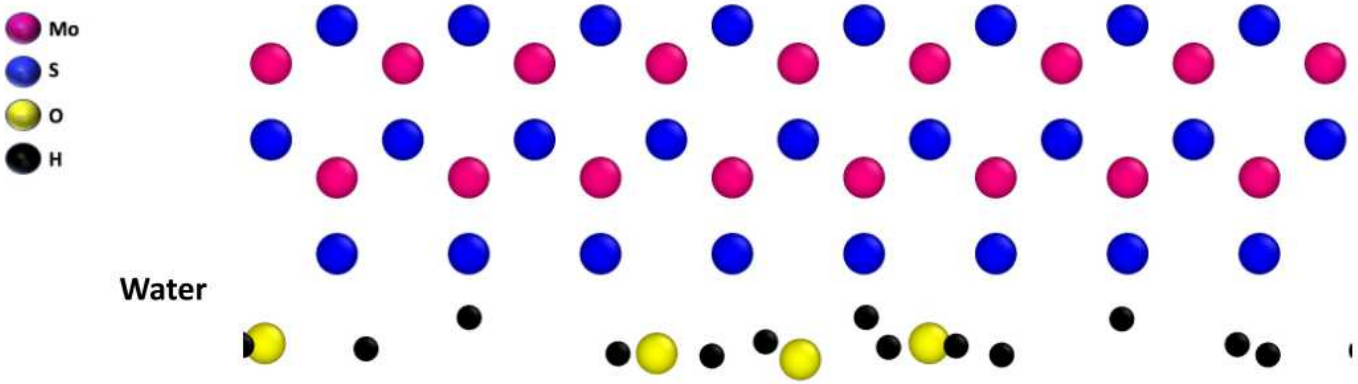
Defects: Added S (66.8% S, 33.2% Mo) with Oxygen



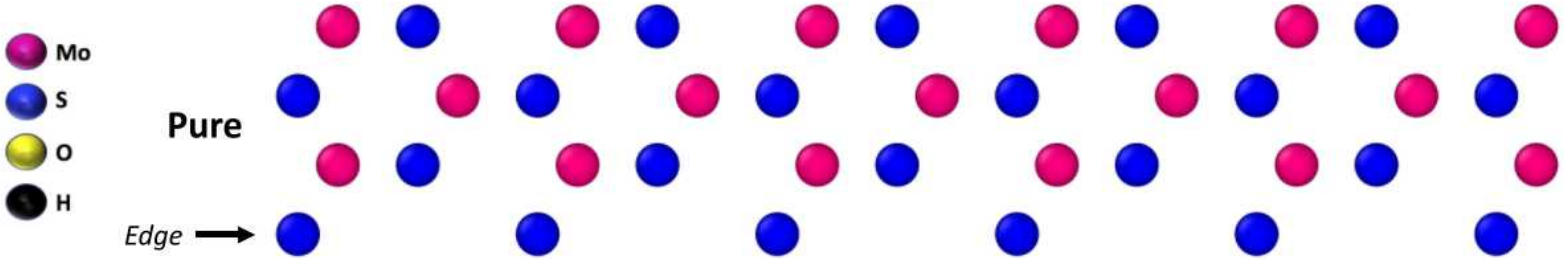


Defects: Added S (66.8% S, 33.2% Mo) with H_2O

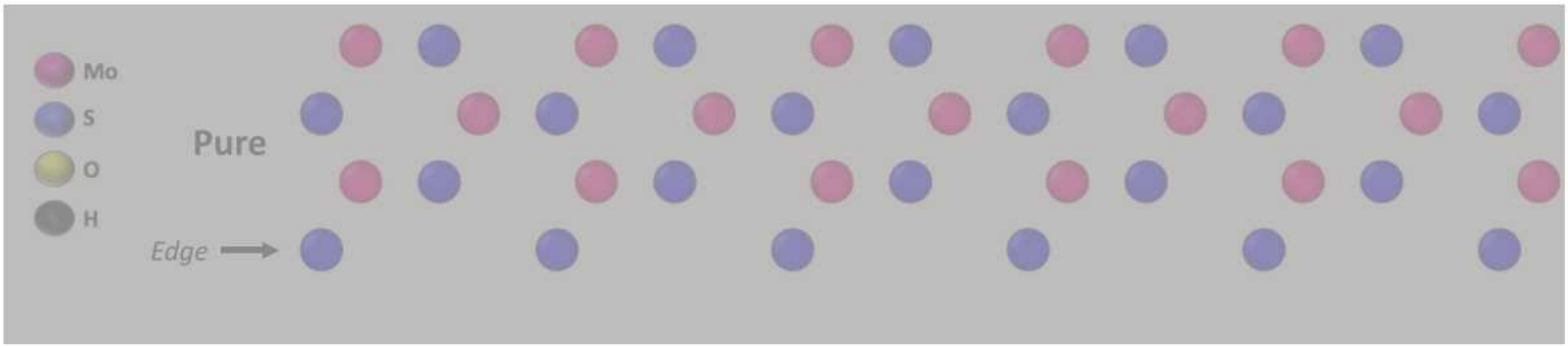


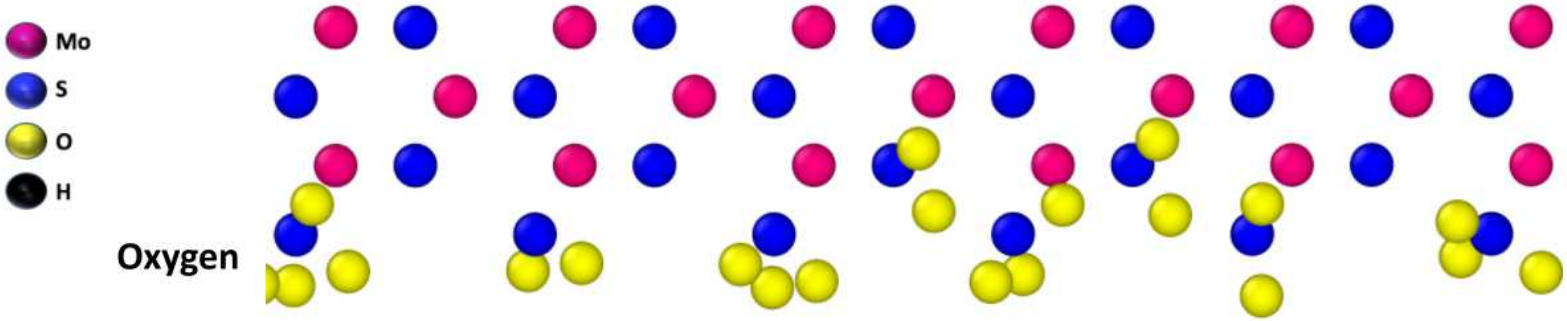


Defects: Mo removed (67.0% S, 33.0% Mo)

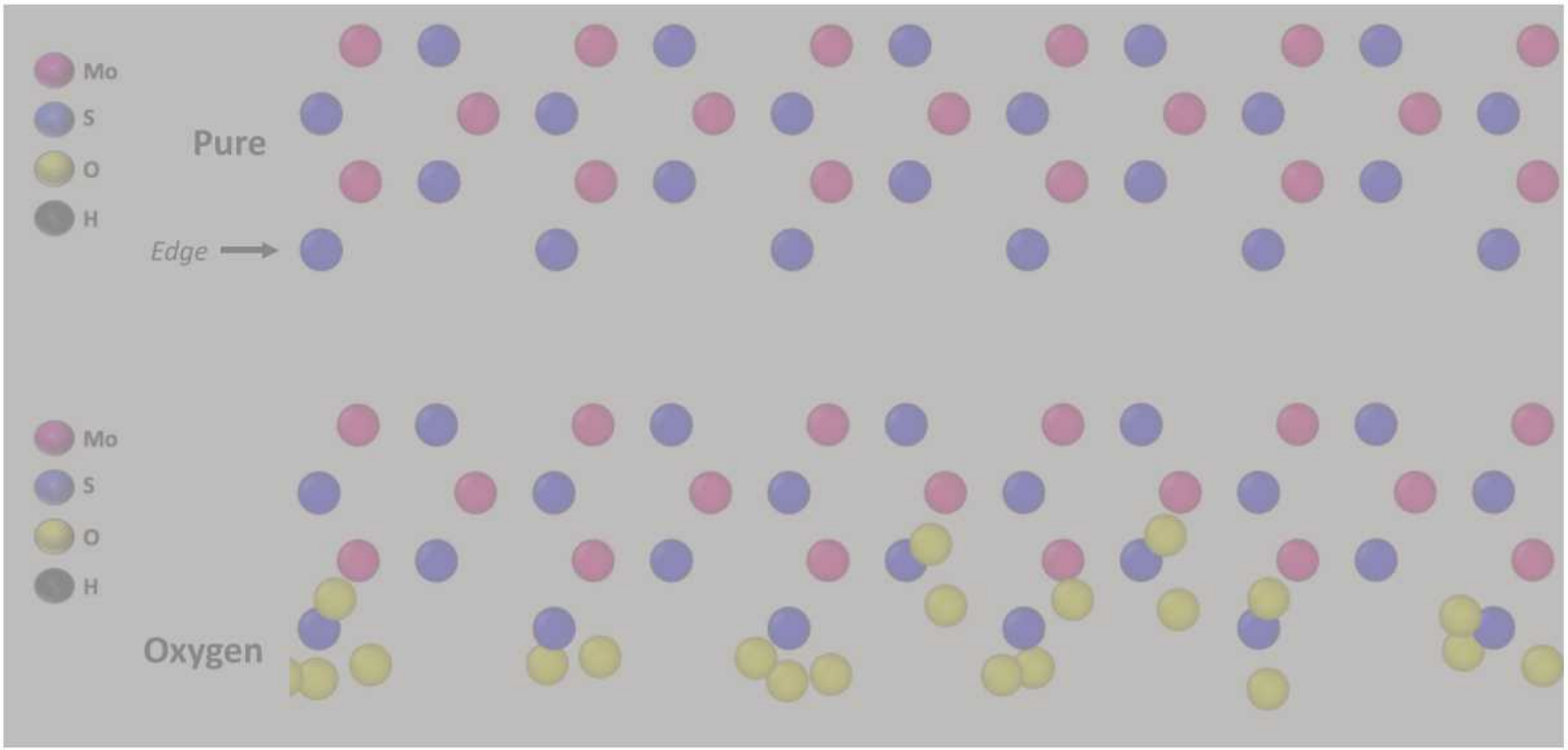


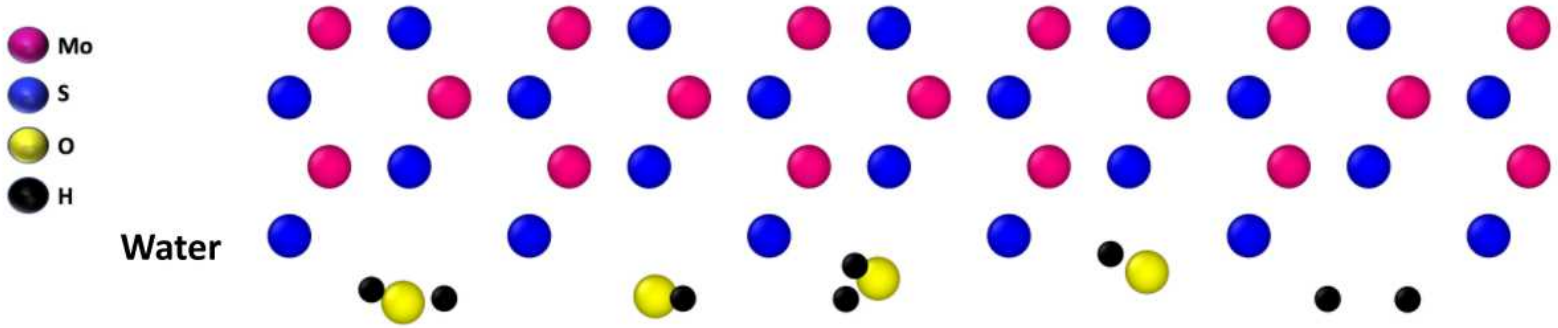
Defects: Mo removed (67.0% S, 33.0% Mo) with Oxygen



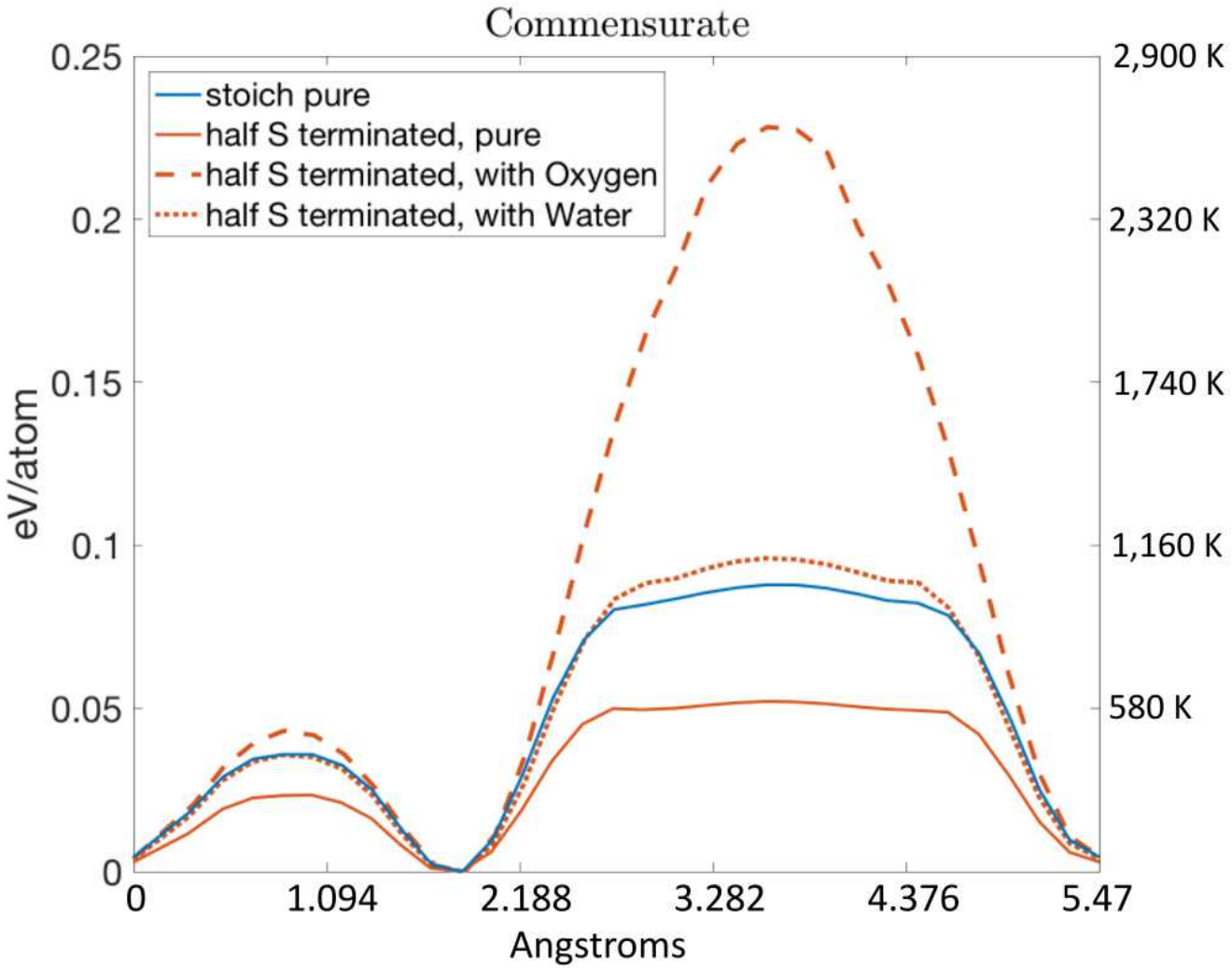


Defects: Mo removed (67.0% S, 33.0% Mo) with H_2O

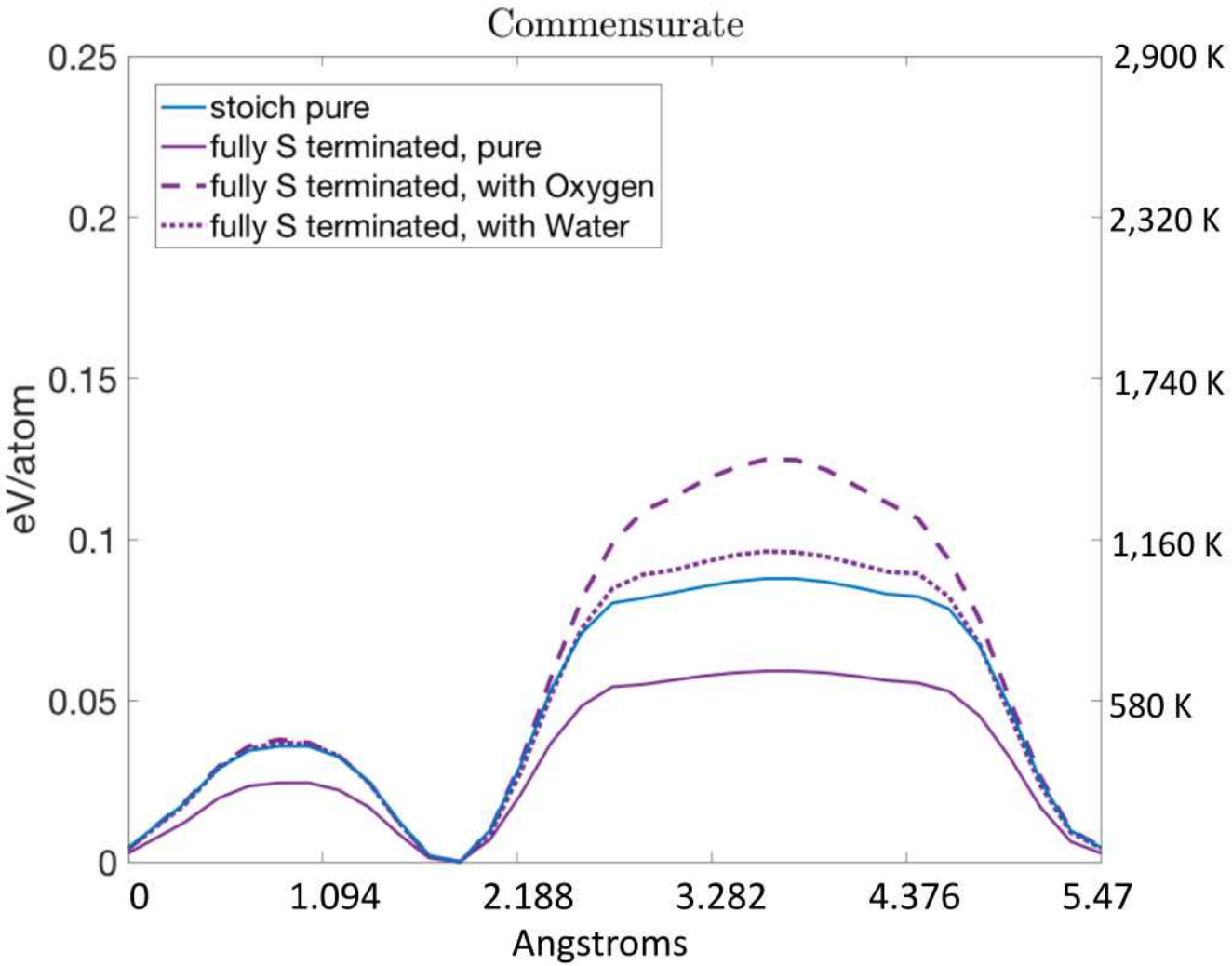




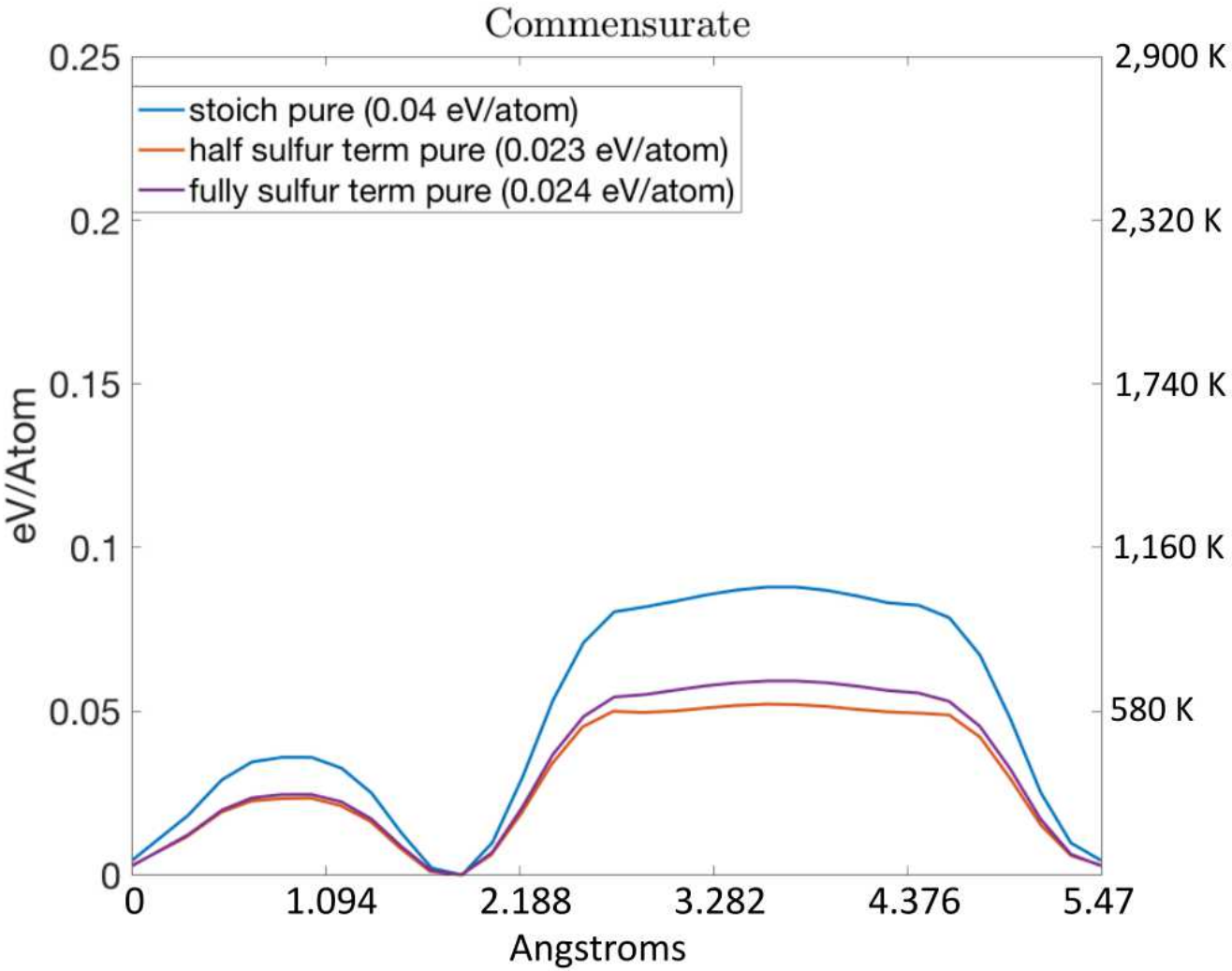
Effect of Water on Friction of MoS_2



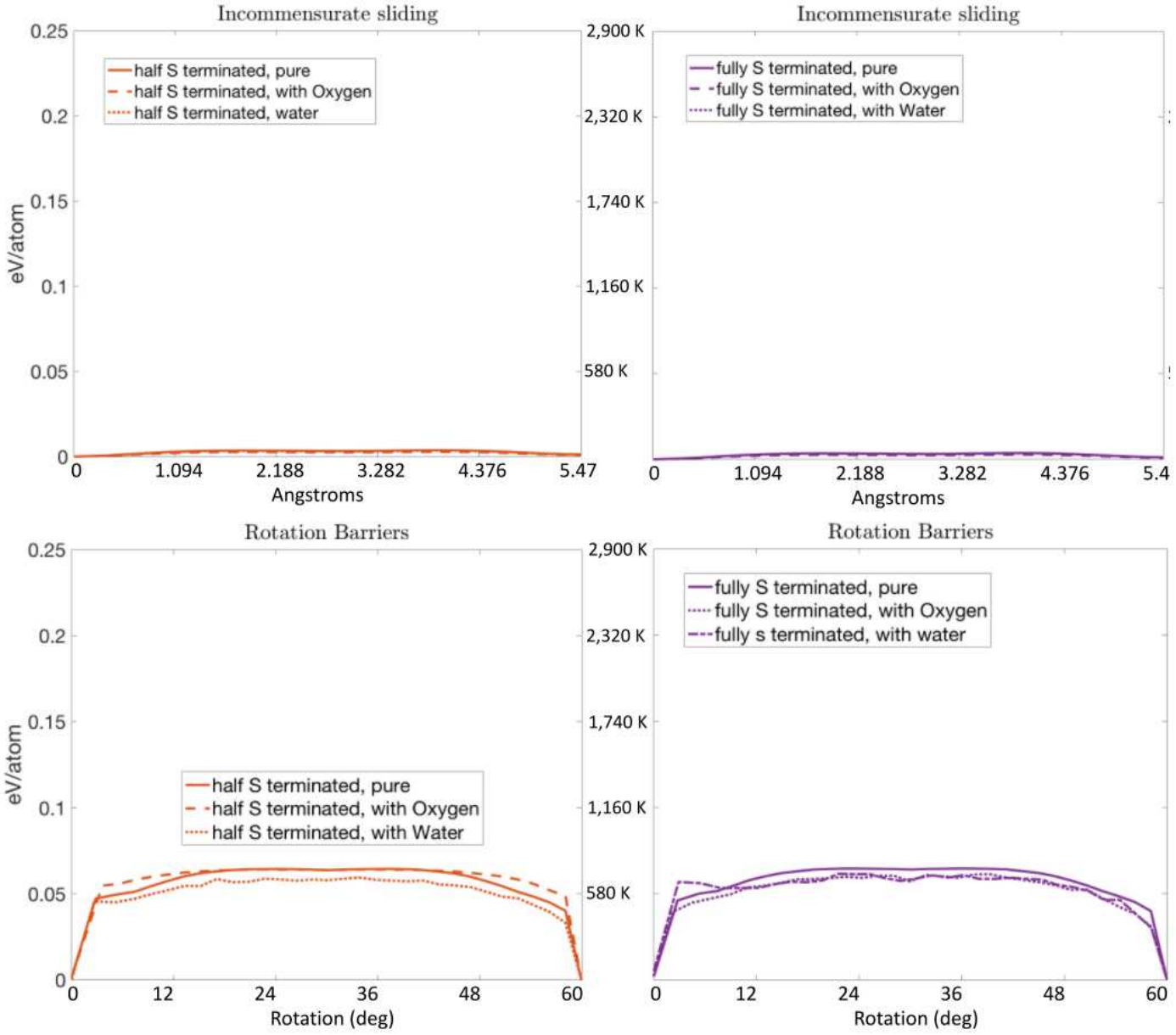
Effect of Water on Friction of MoS_2



Effect of Water on Friction of MoS_2



Effect of Water on Friction of MoS_2



Effect of Water on Friction of MoS_2

- Defects (edge changes) affect barrier far more than $H_2O/O_2/O$ around edges, but only commensurate barrier.
- Water between flake and substrate; possible "third body effect"

  G. He, M.M. Müser, M.O. Robbins, Science, 284 (1990).
- DFT/MD calculations with Quentarius Moore (DOE CSGF Fellow, Texas A&M).
- Effect of strain/deformation on chemistry and reactivity with environment.

Effect of Water on Friction of MoS_2

- Defects (edge changes) affect barrier far more than $H_2O/O_2/O$ around edges, but only commensurate barrier.
- Water between flake and substrate; possible "third body effect"

  G. He, M.M. Müser, M.O. Robbins, Science, 284 (1990).
- DFT/MD calculations with Quentarius Moore (DOE CSGF Fellow, Texas A&M).
- Effect of strain/deformation on chemistry and reactivity with environment.

Effect of Water on Friction of MoS_2

- Defects (edge changes) affect barrier far more than $H_2O/O_2/O$ around edges, but only commensurate barrier.
- Water between flake and substrate; possible "third body effect"

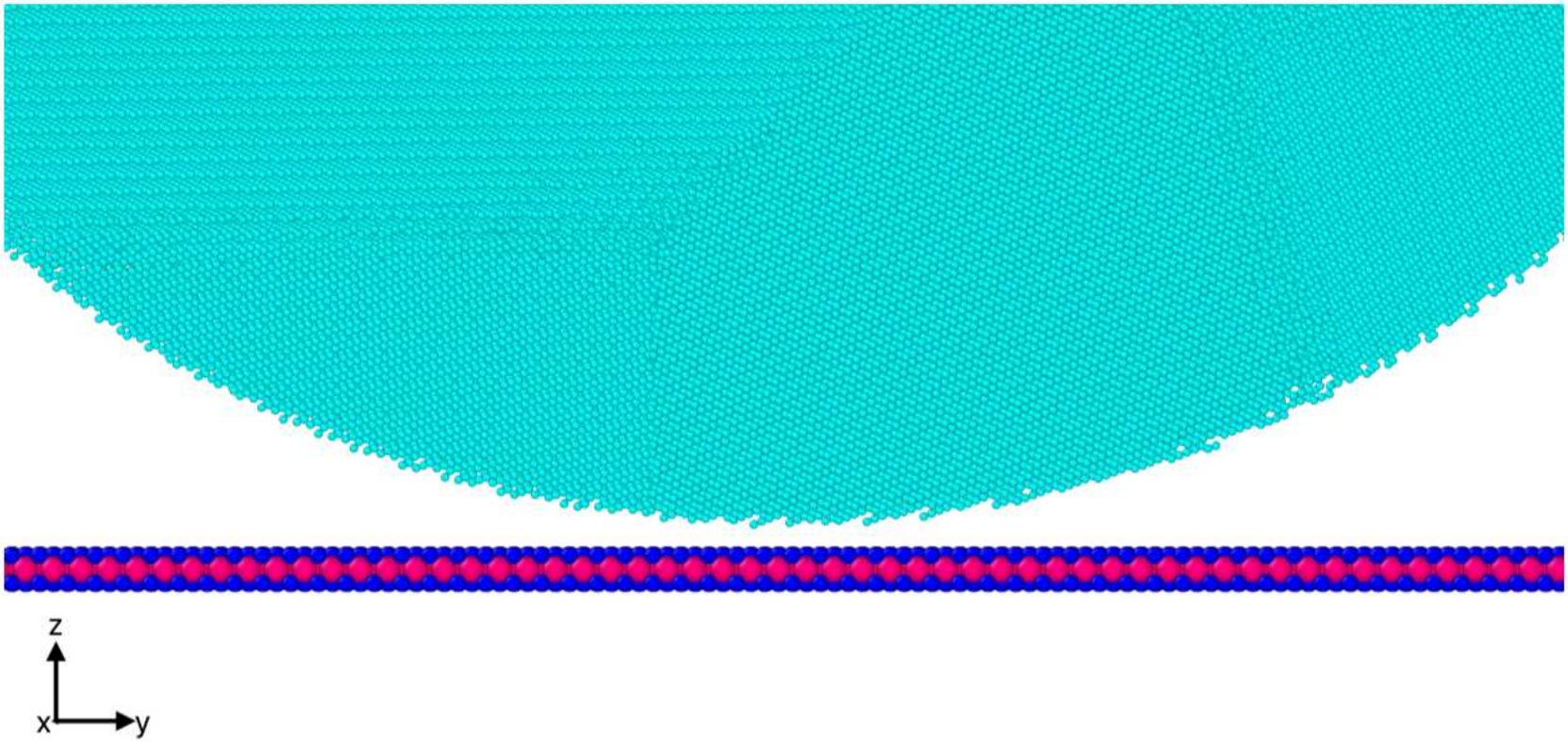
  G. He, M.M. Müser, M.O. Robbins, Science, 284 (1990).
- DFT/MD calculations with Quentarius Moore (DOE CSGF Fellow, Texas A&M).
- Effect of strain/deformation on chemistry and reactivity with environment.

Effect of Water on Friction of MoS_2

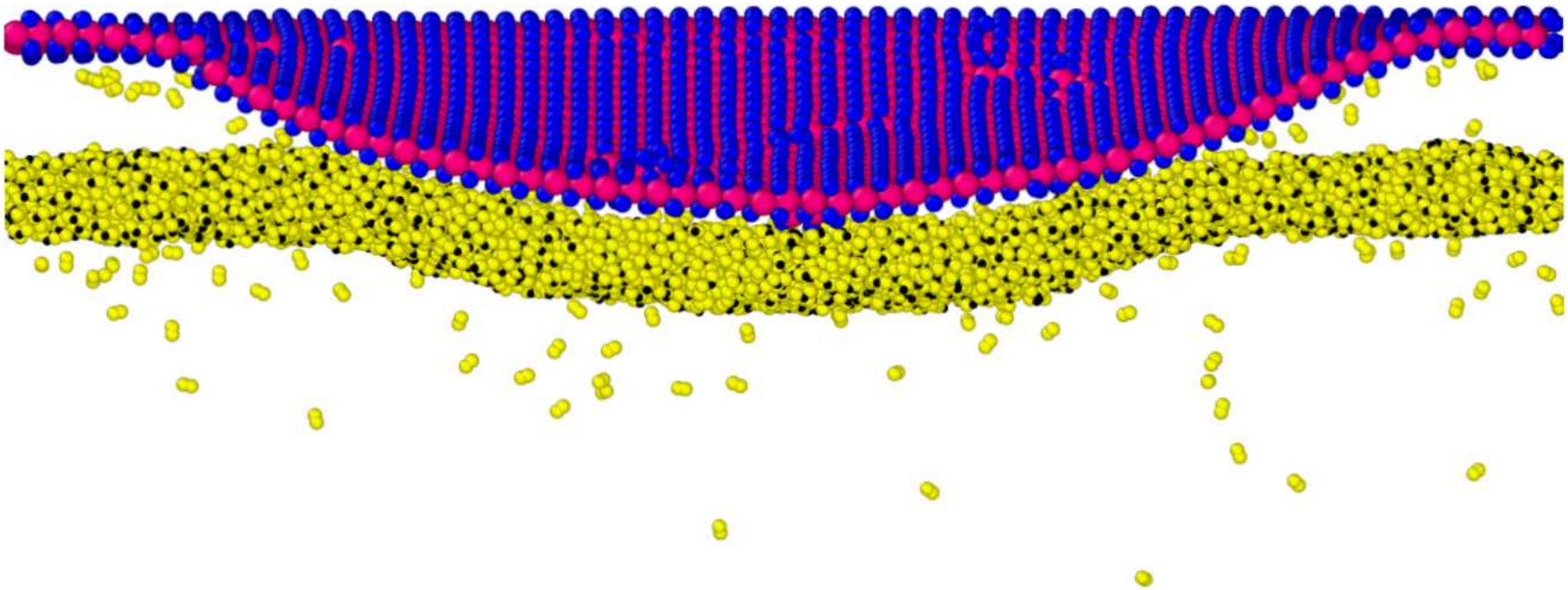
- Defects (edge changes) affect barrier far more than $H_2O/O_2/O$ around edges, but only commensurate barrier.
- Water between flake and substrate; possible "third body effect"

  G. He, M.M. Müser, M.O. Robbins, Science, 284 (1990).
- DFT/MD calculations with Quentarius Moore (DOE CSGF Fellow, Texas A&M).
- Effect of strain/deformation on chemistry and reactivity with environment.

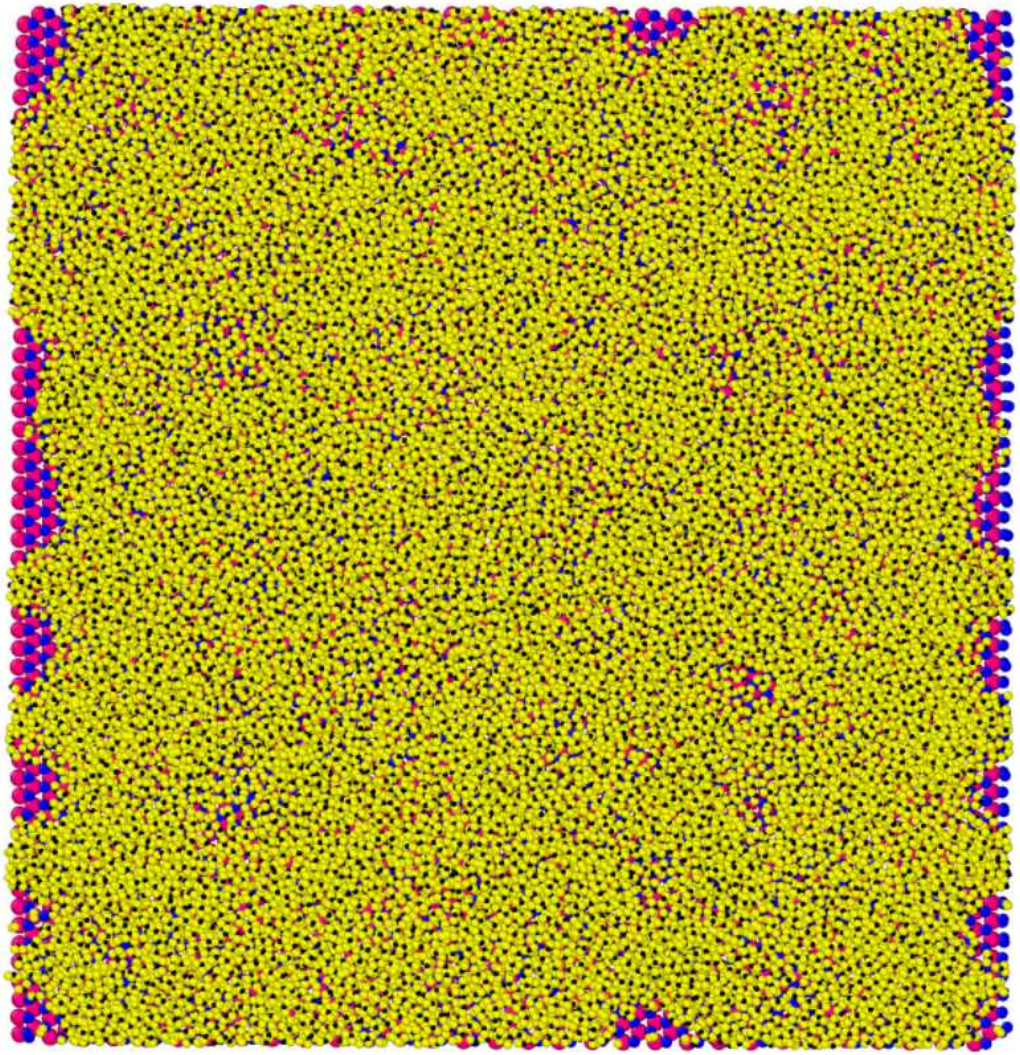
Indentation of MoS_2



Strained MoS_2 and increased reactivity?



Strained MoS_2 and increased reactivity? Accelerated MD?



Acknowledgements & Questions

- Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and 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.