SAND2019-5729C

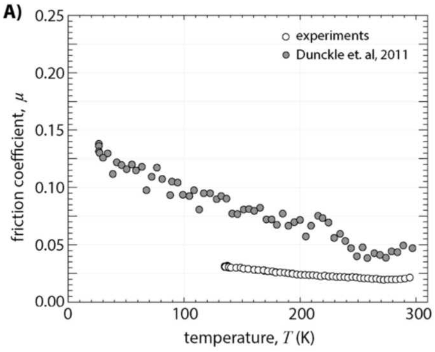
Towards a Model of Friction for MoS2 in the Presence of Environment and Defects

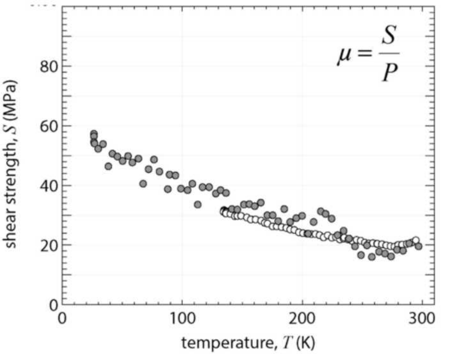
Adam R. Hinkle, John F. Curry, Tomas F. Babuska, Michael T. Dugger, Mark A. Wilson, Brandon A. Krick, Nicolas Argibay, and Michael Chandross

Sandia National Laboratories, Albuquerque, NM, USA

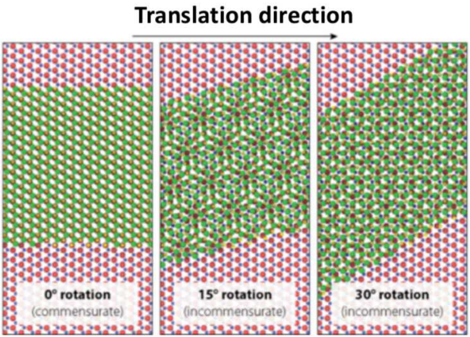
STLE 2019

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





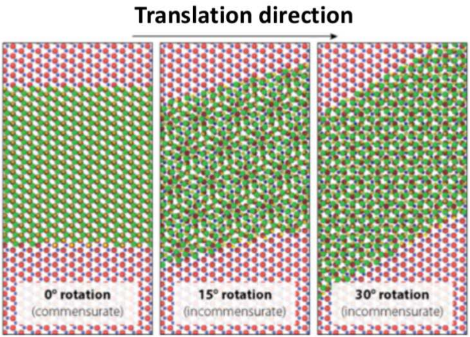
Nudged Elastic Band Calculations and Commensurate Sliding

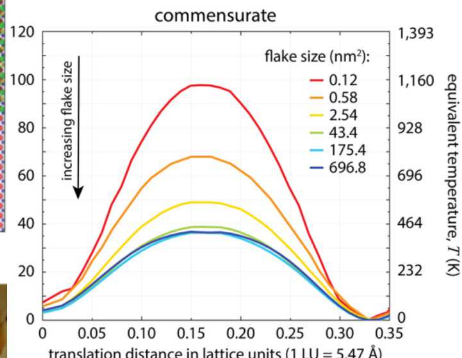



commensurate
egg shell


incommensurate
egg shell

Nudged Elastic Band Calculations and Commensurate Sliding

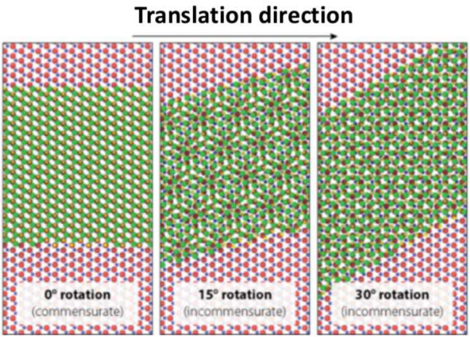


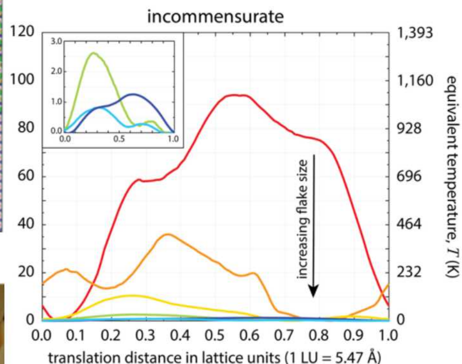


commensurate egg shell

incommensurate egg shell

Rotation Barrier

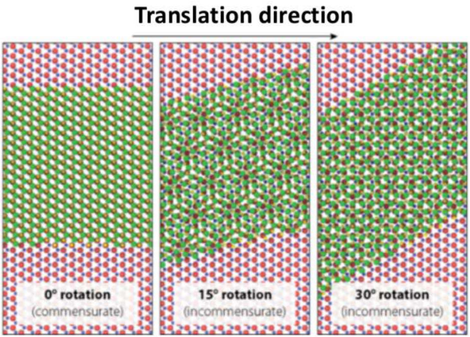




commensurate
egg shell

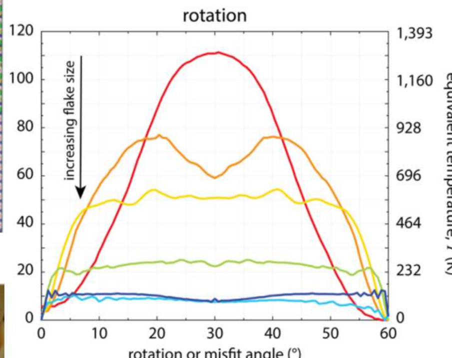
incommensurate
egg shell

Incommensurate Barrier

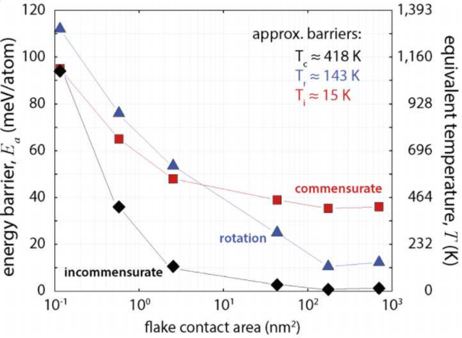


commensurate
egg shell

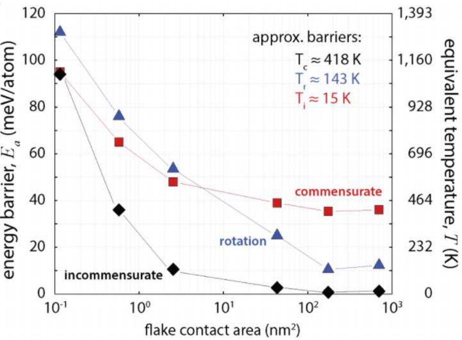
incommensurate
egg shell



A Toy Model in terms of energy barriers (mechanisms to sliding)



A Toy Model in terms of energy barriers (mechanisms to sliding)



The probability and failure to overcome a barrier n

$$p_n = A \exp\left(\frac{-\Delta E_n}{k_B T}\right)$$

$$f_n = 1 - p_n$$

The probability to slide and fail to slide (friction):

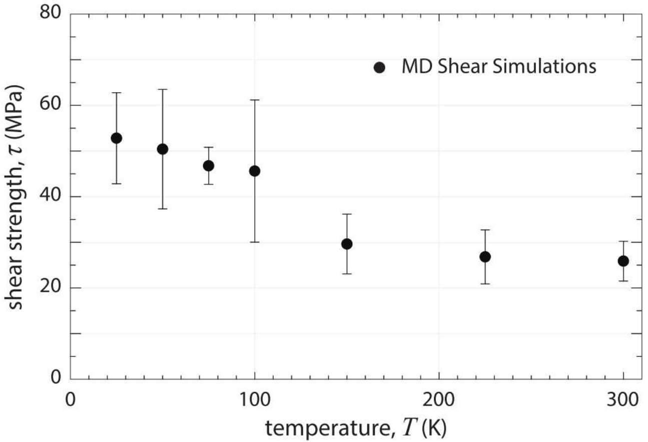
$$p_{slide} = p_r p_i + f_r p_c$$

$$f_{slide} = 1 - p_{slide}$$

$$= 1 - (p_r p_i + f_r p_c)$$

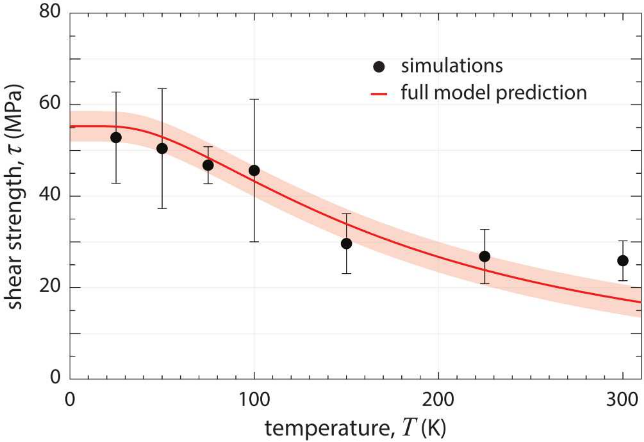
The model and data from $S(T) = S_L f_{slide}(T)$

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



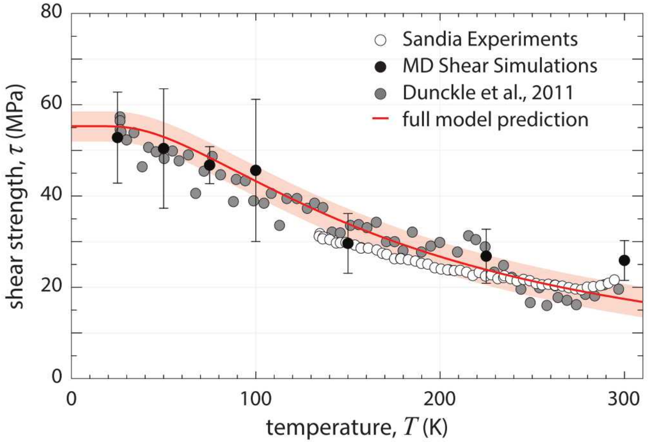
The model and data from $S(T) = S_L f_{slide}(T)$

$$S_L = 55.3 \text{ MPa}$$



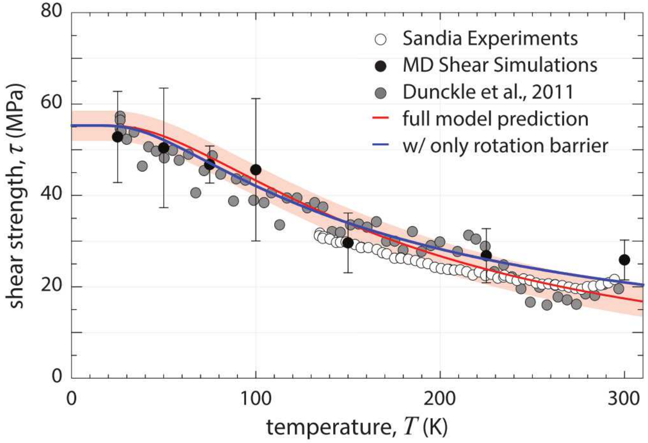
The model and data from $S(T) = S_L f_{slide}(T)$

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



The model and data from $S(T) = S_L f_{slide}(T)$

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



Letter available now online

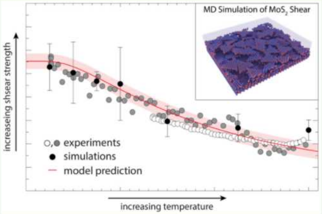
ACS APPLIED NANO MATERIALS
Letter
Cite This: ACS Appl. Nano Mater. XXXX, XXX, XXX–XXX
www.acsanm.org

Atomistic Origins of Temperature-Dependent Shear Strength in 2D Materials

John F. Curry,[†,‡] Adam R. Hinkle,[†,‡] Tomas F. Babuska,[†,§] Mark A. Wilson,[†] Michael T. Dugger,[†] Brandon A. Krick,[§] Nicolas Argibay,[*,†] and Michael Chandross[*,†]

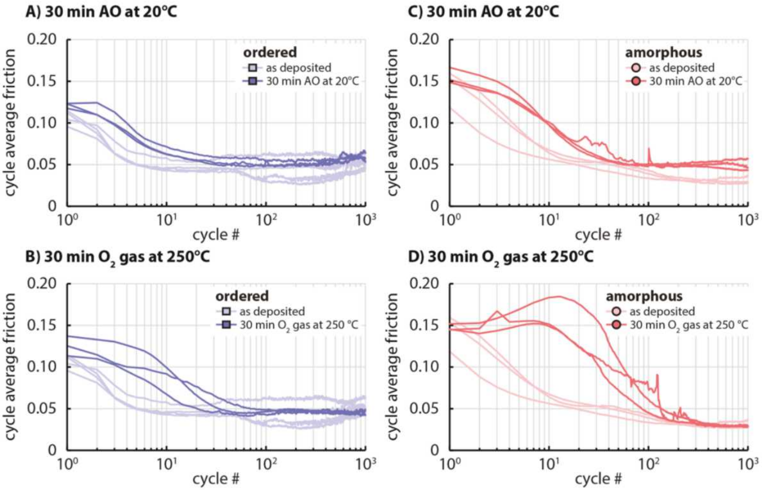
[†]Material, Physical and Chemical Sciences Center, Sandia National Laboratories, Albuquerque, New Mexico 87123, United States
[§]Department of Mechanical Engineering & Mechanics, Lehigh University, Bethlehem, Pennsylvania 18015, United States

ABSTRACT: We present a model that predicts the macroscale temperature-dependent interfacial shear strength of 2D materials like MoS_2 based on atomistic mechanisms and energetic barriers to sliding. Atomistic simulations were used to systematically determine the lamellar size-dependent rotation and translation energy barriers, that were used to accurately predict a broad range of experimental data. This framework provides insight about the origins of characteristic shear strengths of 2D materials.

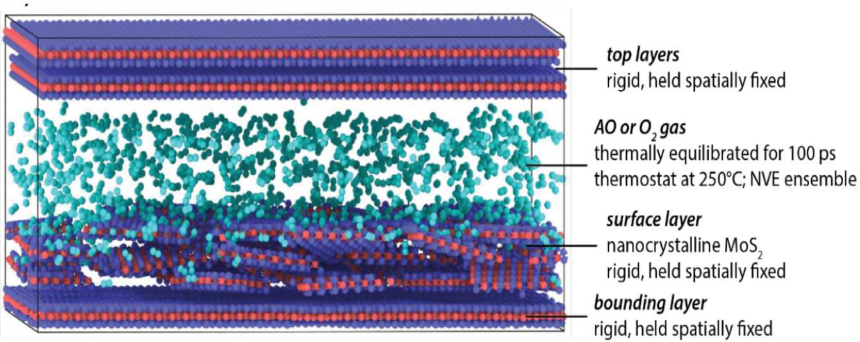


KEYWORDS: *2D materials, MoS_2, molybdenum disulfide, nudged elastic band, superlubricity, molecular dynamics, activation energy, temperature*

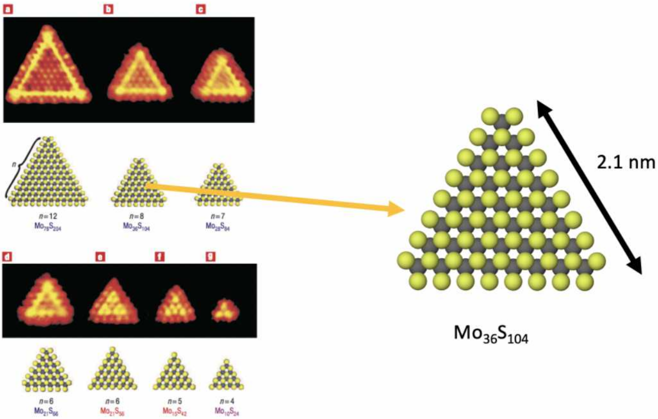
Amorphous and orderd friction in Oxygen



Molecular Dynamics Simulations



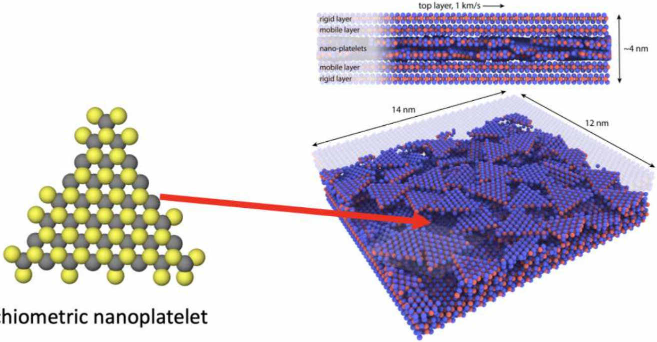
MoS_2 platelets



Lauritsen et al., Nature Nanotech. 2007

- Start with nanoplatelets
- Defect free platelets are non-stoichiometric

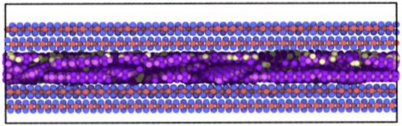
MoS_2 platelets

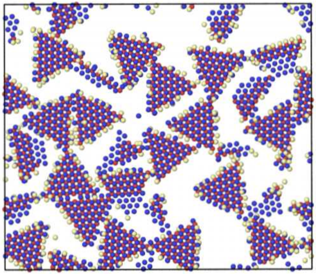


stoichiometric nanoplatelet

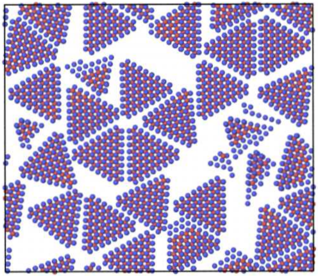
- Sandwich 64 nanoplatelets
  - Mobile lamella on top & bottom
  - Fixed lamella (rigid layer) to control load and speed
- ReaxFF: Vasenkov, et al., J. Appl. Phys. 2012

Interplatelet bonding



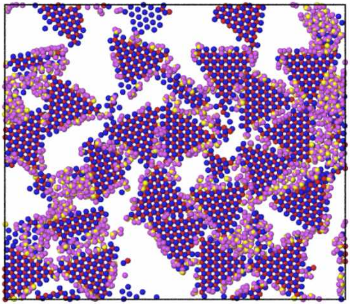


oxygen passivated

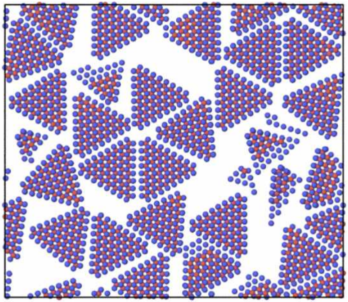


defect free

Interplatelet bonding

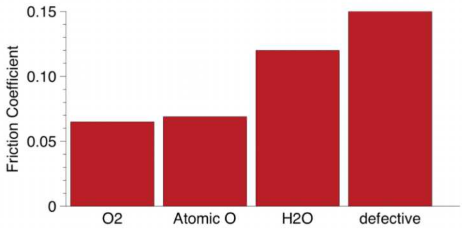


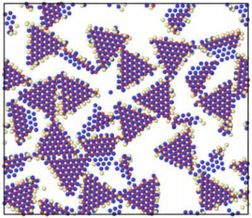
water passivated



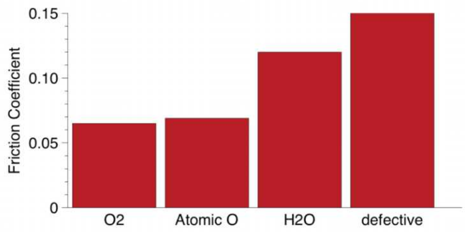
defect free

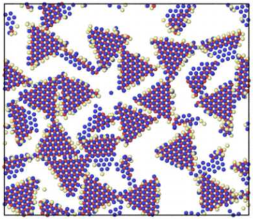
Friction: Defective vs. Non-Defective

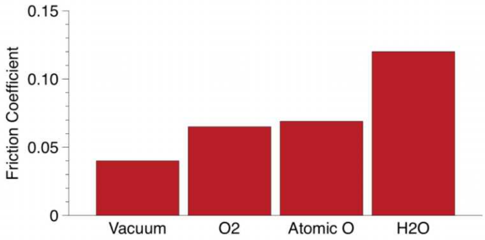




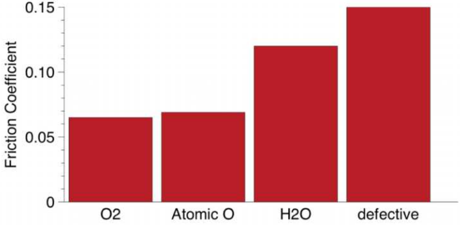
Friction: Defective vs. Non-Defective

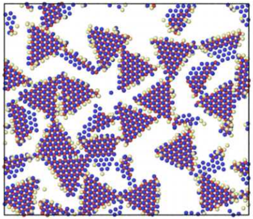


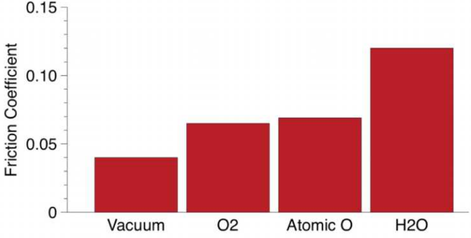


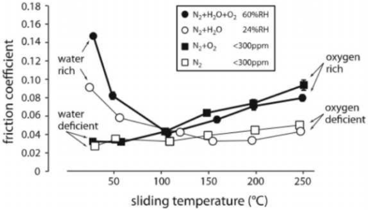


Friction: Defective vs. Non-Defective

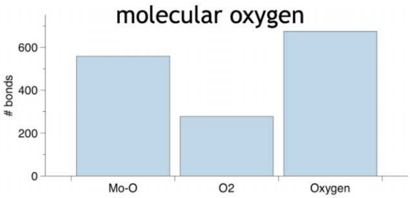


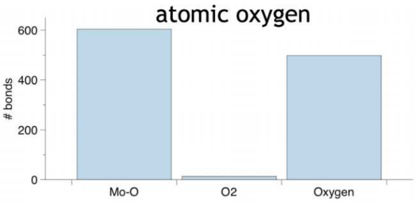


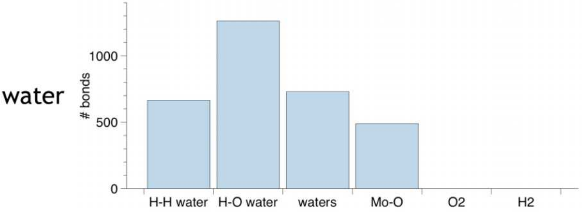




Chemistry via bonds

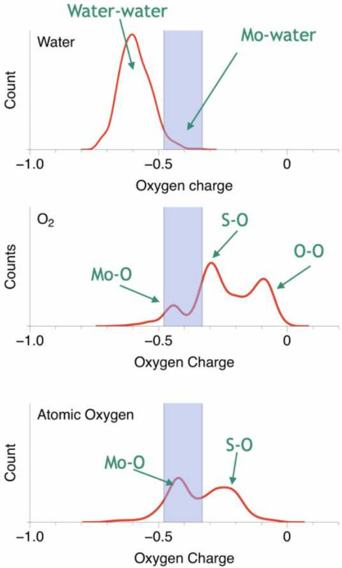


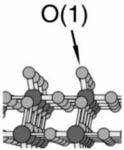




- Water does not dissociate (no O2 or H2 formed)
- Molecular O shows little dissociation (mostly in O2)
- Atomic oxygen forms little O2

Chemistry confirmed by partial charges

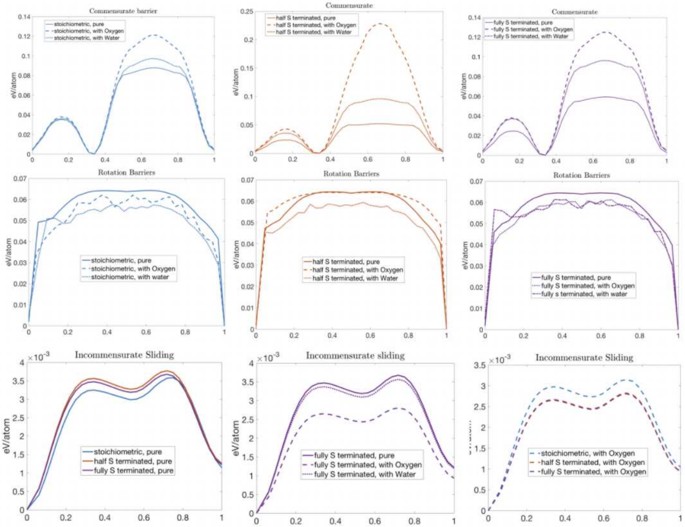




Tokarz-Sobieraj et al.
Surf. Sci. 2001

- Oxygen bonded to Mo has partial charge from -0.48 (Tokarz-Sobieraj et al. Surf. Sci. 2001) to -0.33 (Yin et al., J. Mol. Model 2001).
- Oxygen in water has partial charge from -0.6 to -0.8(Astrand, et al., J. Phys. Chem. A 1998).
- Water shows only physisorption
- Atomic oxygen shows chemisorption
- Molecular oxygen shows slight amount of chemisorption

Barriers: Environment vs. Defects



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.

- James Batteas, Department of Chemistry, Texas A&M University, College Station

Sandia National Laboratories U.S. DEPARTMENT OF ENERGY