Analyzing the Efficacy of a Janus Rippled Atomic Structure for use in the Hydrogen Evolution Reaction via Density Functional Theory Calculations

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Background

- Global warming poses an existential threat to humanity. Just in 2018 alone, burning fossil fuels for energy caused 76% of the U.S.'s greenhouse gas emissions [1].
- A better method of energy generation would be to burn hydrogen gas where the only byproduct is water.
- One promising way to produce hydrogen gas is through the Hydrogen Evolution Reaction (HER).
- The HER reaction occurs when a plate is submerged in water then a current is run through it. An important aspect of this scenario is the surface chemistry of the plate.
- Specifically, the surface chemistry of the plate should have a Gibbs free energy (ΔG_H) strong enough to take hydrogen from the water, but weak enough to release the hydrogen for collection [2,3].
- Two ways to influence the surface chemistry is to explore the Janus and rippled atomic structures. A Janus structure means that an atomic structure is asymmetric, and a rippled structure means that the atomic structure in the longitudinal direction follows a "rippled" shape [4,5].
- This FURI project seeks to find an optimal atomic structure that would meet the favorable HER criteria using Janus and rippled atomic structures.

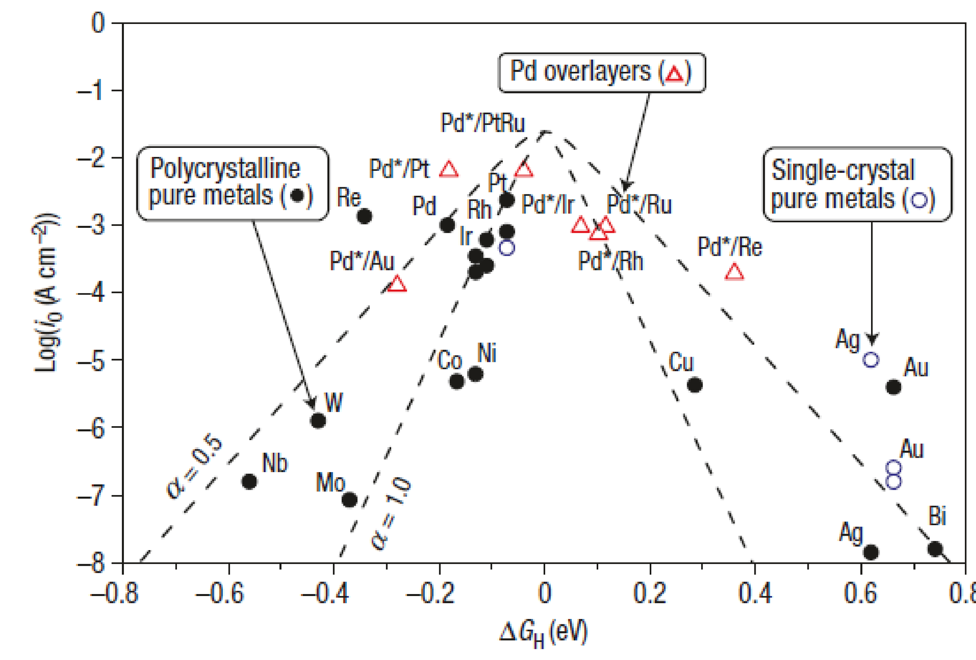

Figure 1. Volcano Plot for the HER for various pure metals and metal overlayers [3].

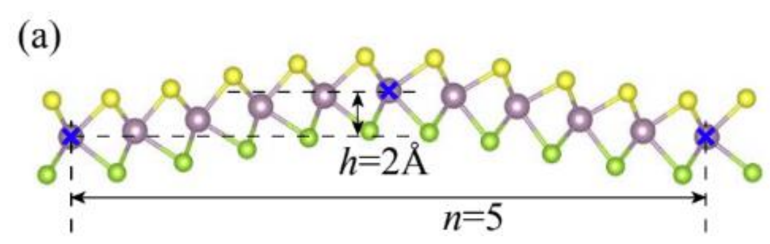

Figure 2. Atomic Structure in the x-y plane displaying a slight ripple.

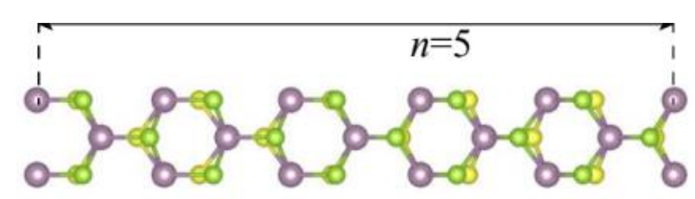

Figure 3. The same structure displaying Janus features in the x-z pane.

Research Question

Can a rippled, Janus structure exhibit favorable binding energies for use in HER?

Research Methods and Findings

- First the two Janus, rippled atomic structures in figure 4 were represented via .cif files and displayed through VESTA.
- The two structures were then computationally simulated via DFT to explore whether they exhibited favorable binding energies for HER.
- It can be seen through figure 5 that both structures are able to exhibit the favorable binding energy of 0.08 eV. Future experiments and studies can focus on increasing the area by which this favorable energy is present within the atomic structure.

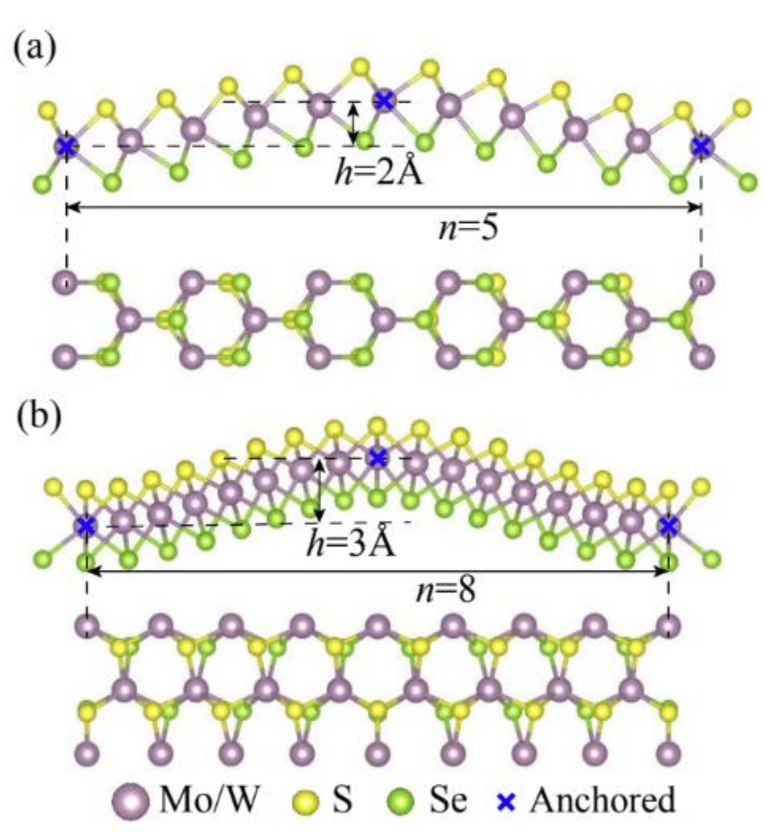

Figure 4. The two structures explored in this project with color-coded element reference.

(a)

n			
5	12	46	103
6	6	24	52
7	4	13	29
8	3	8	18

h (Å)

(b)

n			
5	74	279	580
6	41	158	337
7	24	94	205
8	15	59	130

h (Å)

Color scale: 500, 400, 300, 200, 100

Figure 5. The two structures' binding energy values in mEv.

Acknowledgements and References

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