

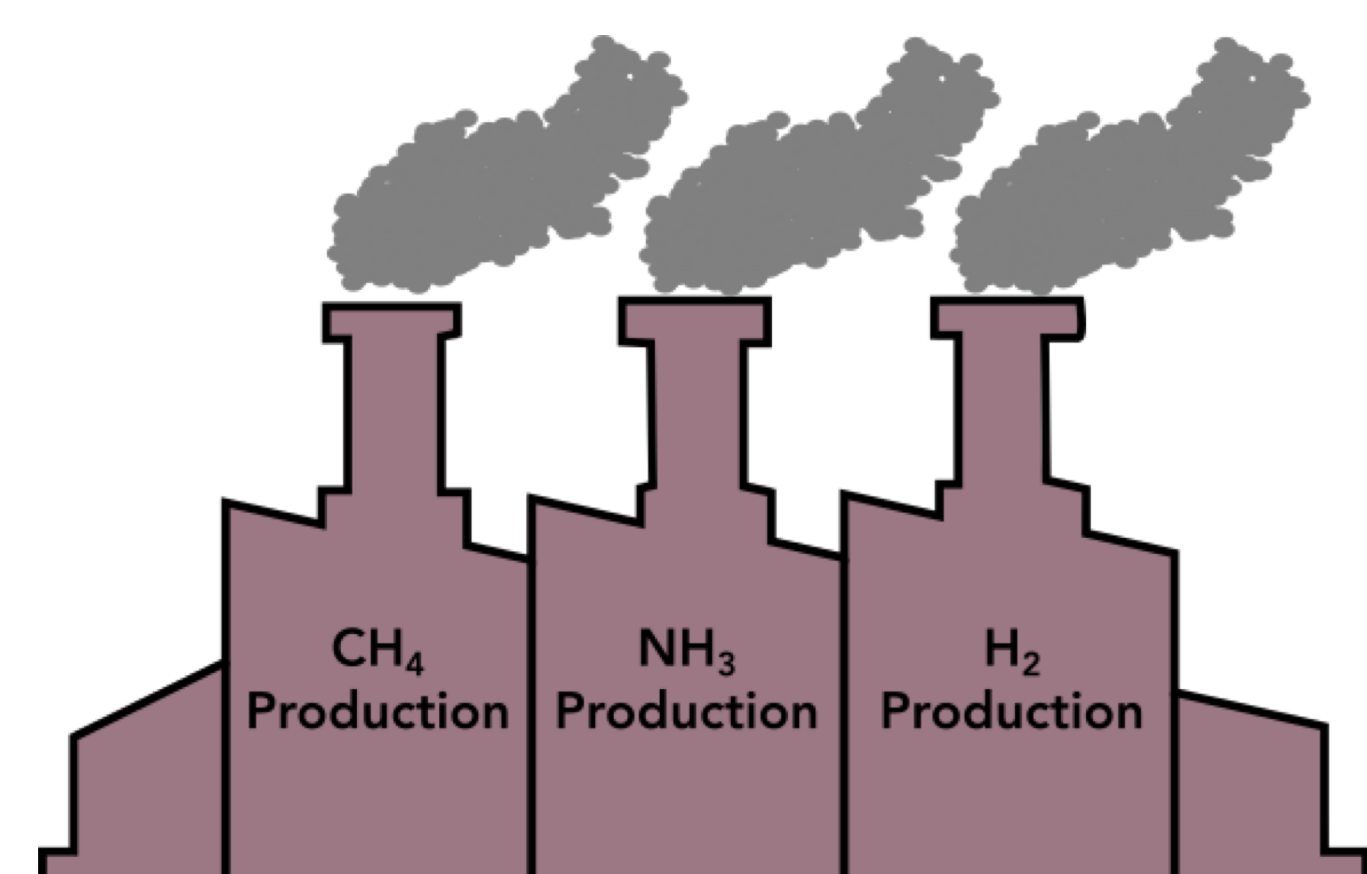
Modeling Solvent and Potential for Electrocatalytic Systems

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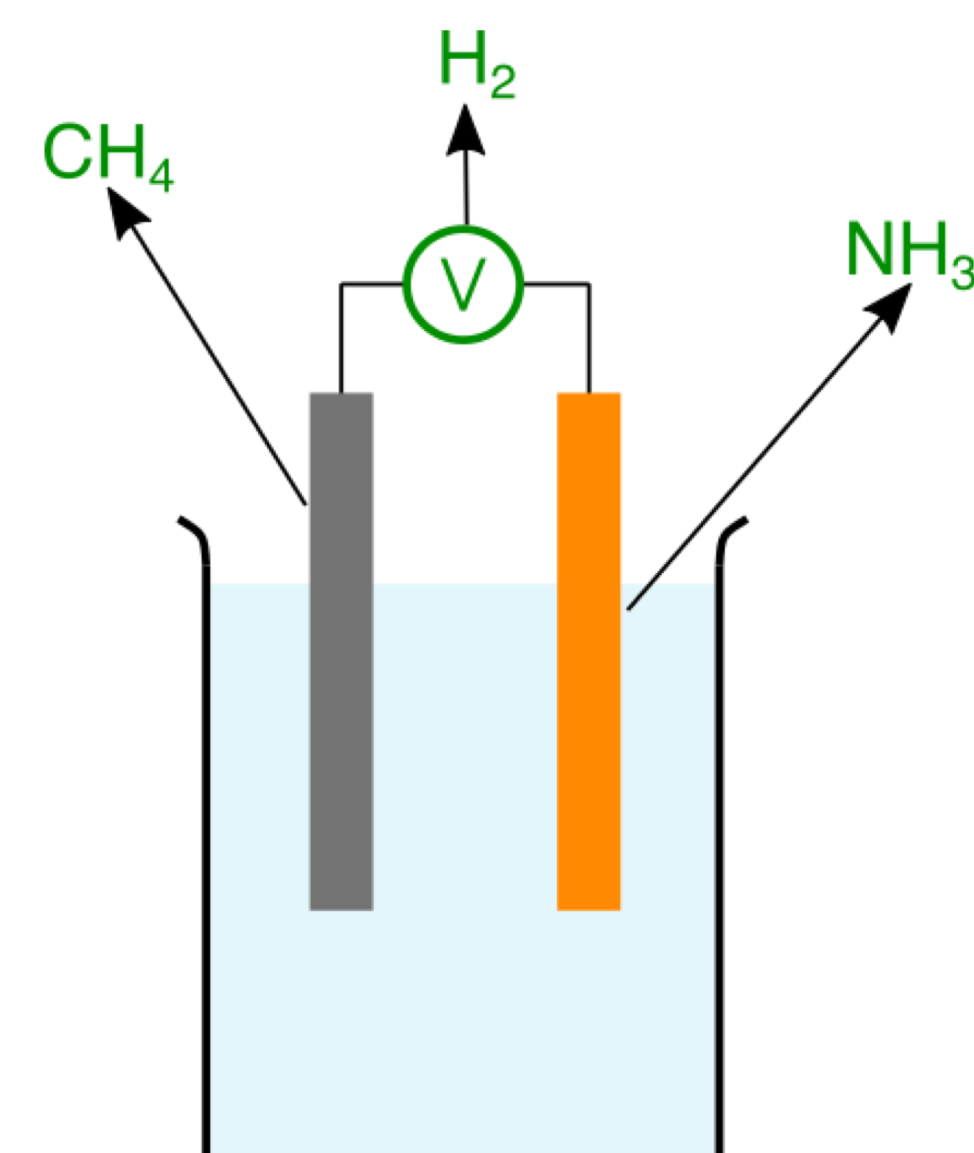
Why Electrocatalysis?

By developing electrocatalytic alternatives to some of the worlds most important chemical reactions we could:

- Reduce the overall **energy cost** of producing critical chemicals such as ammonia and methane.
- Reduce the **production of harmful greenhouse gasses** such as CO₂.
- Move the world to **clean, sustainable and efficient** energy sources like H₂.

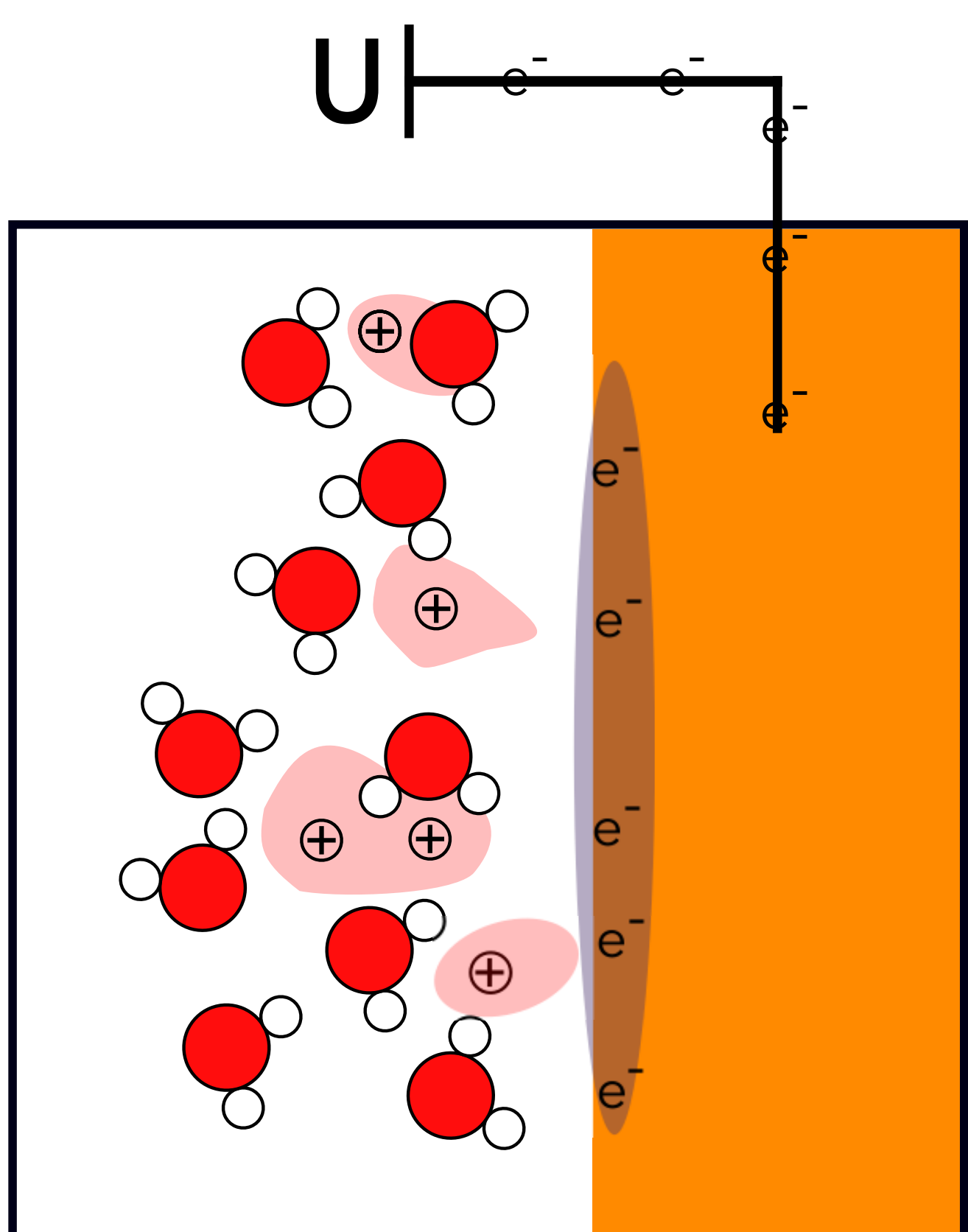


Electrocatalysis



Computational techniques allow for high throughput screening studies to identify the most powerful catalysts. This greatly reduces the material and energy resources required for such research.

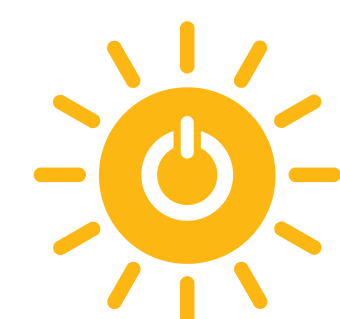
The Challenge that Electrocatalysis Brings



Electrocatalysis requires electricity, or a potential, to work. As shown above this potential can be supplied from renewable sources. However, when it comes to studying electrocatalytic reactions, potential provides two problems:

1. The **energy of the electrons**, crucial to the reactions, is related to the potential.
2. The separation of charge creates a complicated **electrochemical double layer**.

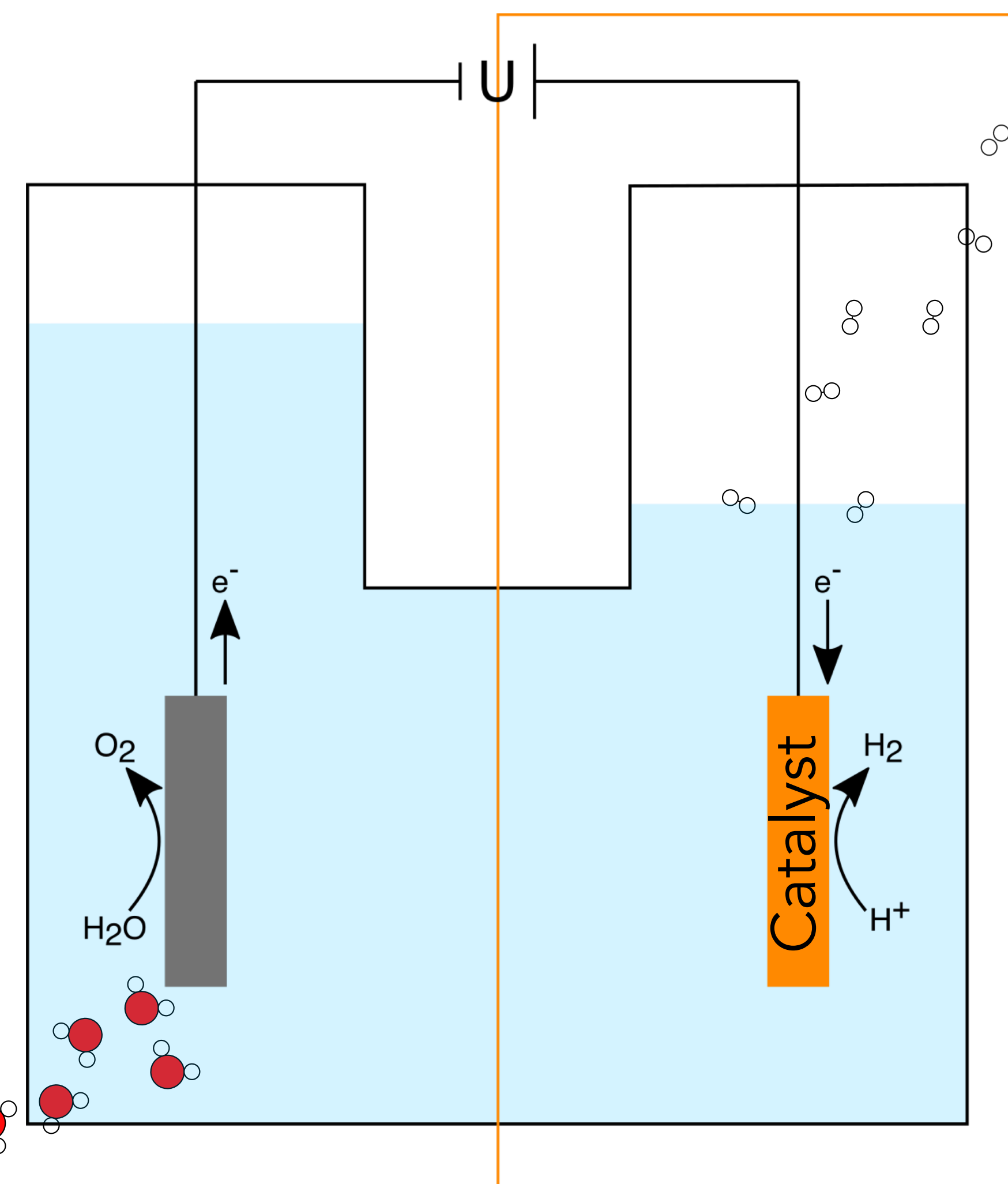
7 AFFORDABLE AND
CLEAN ENERGY



11 SUSTAINABLE CITIES
AND COMMUNITIES



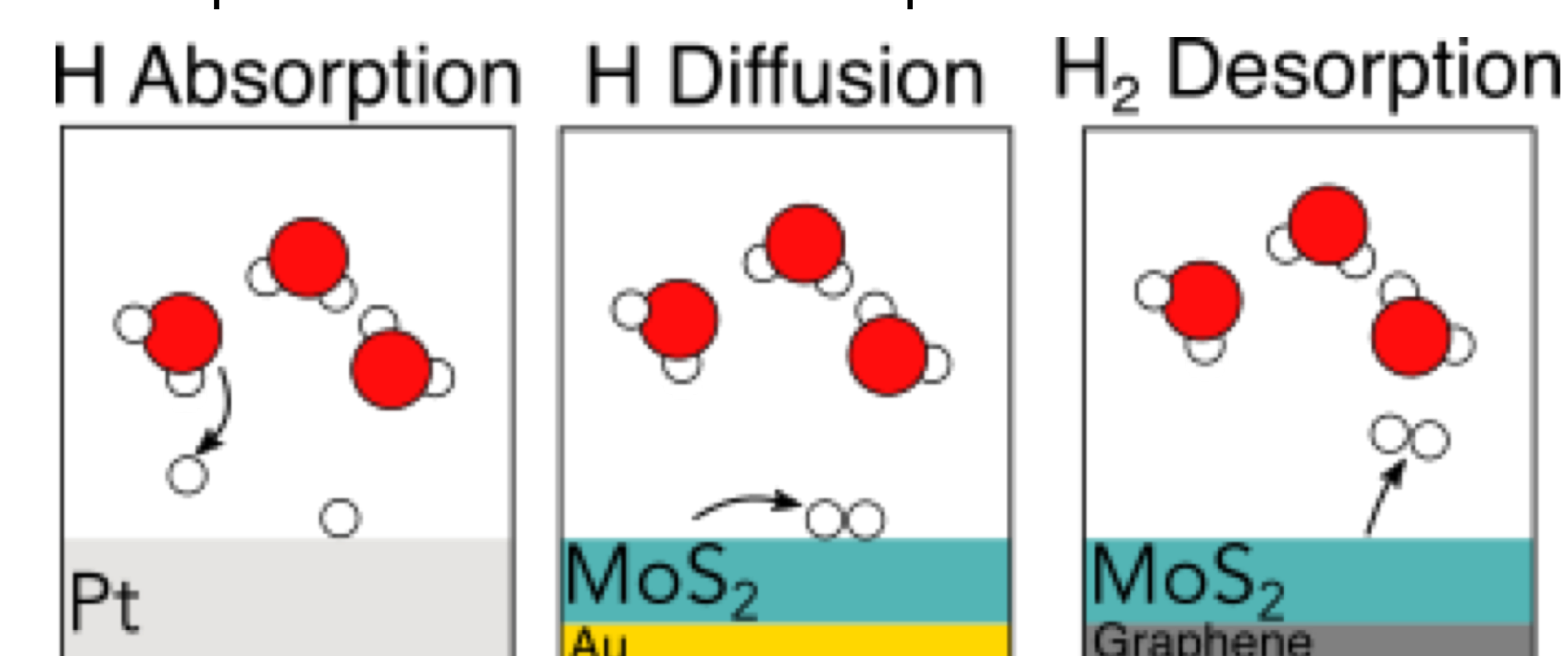
13 CLIMATE
ACTION



The Hydrogen Evolution Reaction (HER)

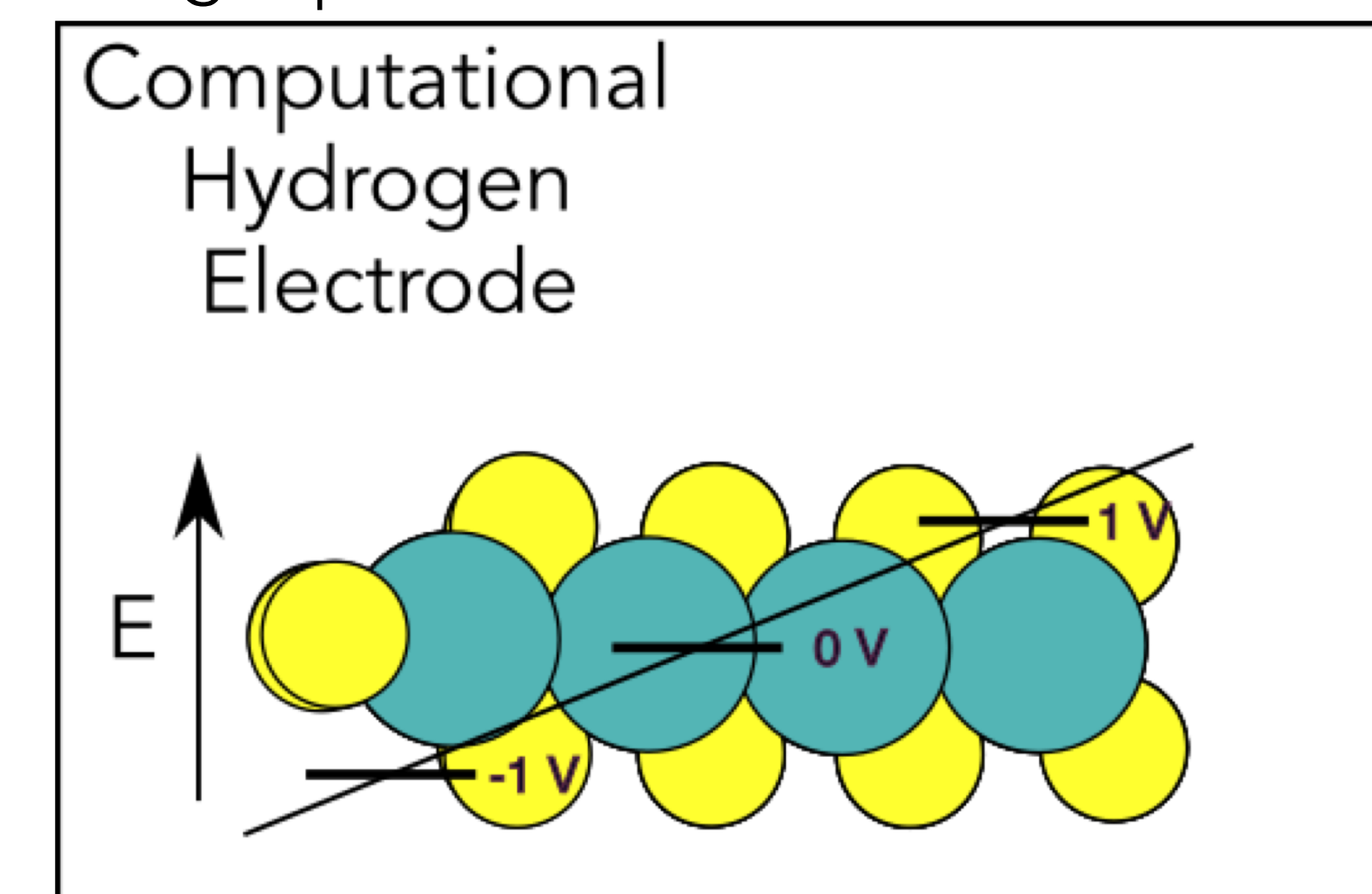
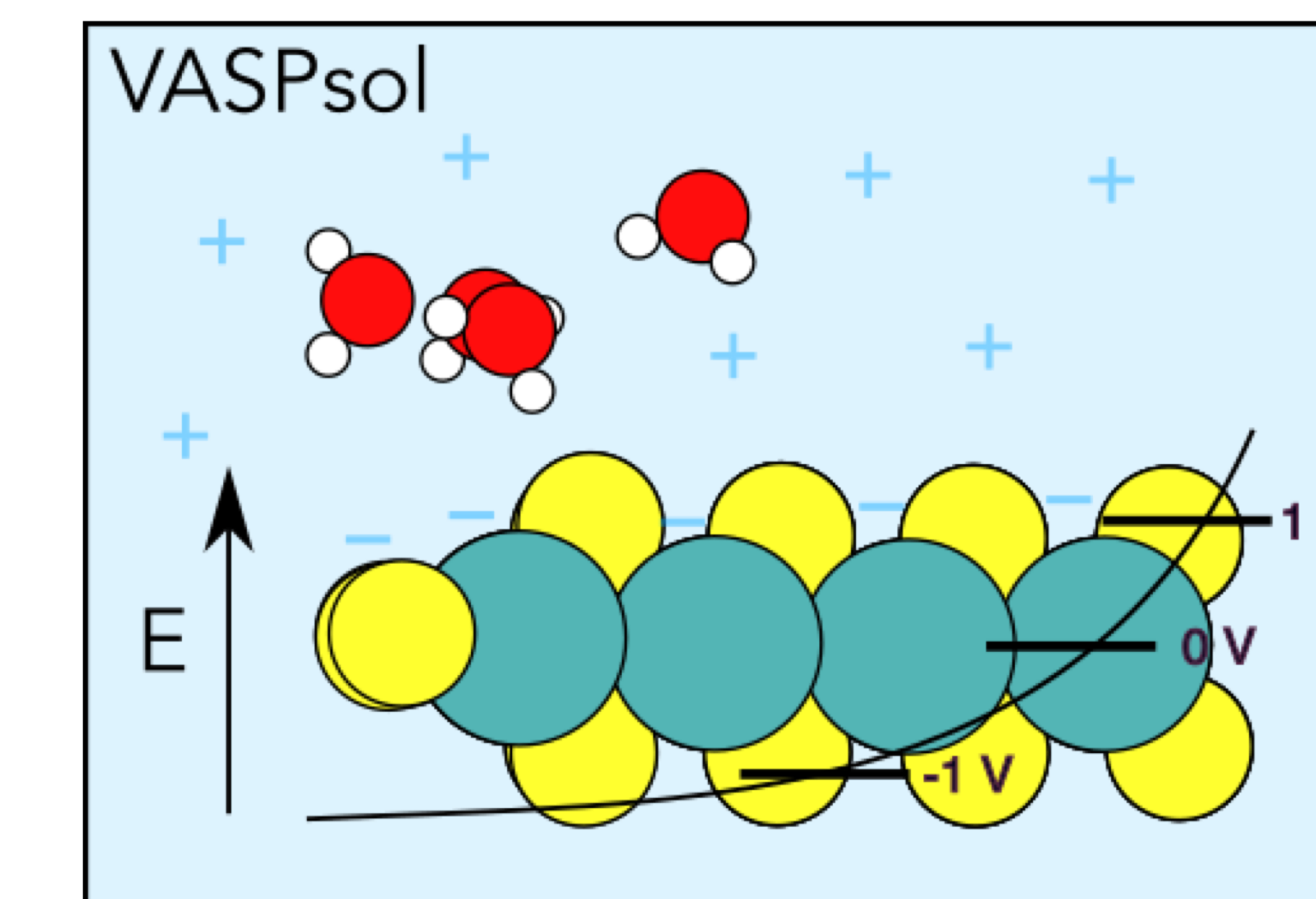


The HER is a simple electrochemical half reaction. The most active catalyst is Pt. However, recent work has shown that MoS₂¹, a cheaper alternative, has promise.



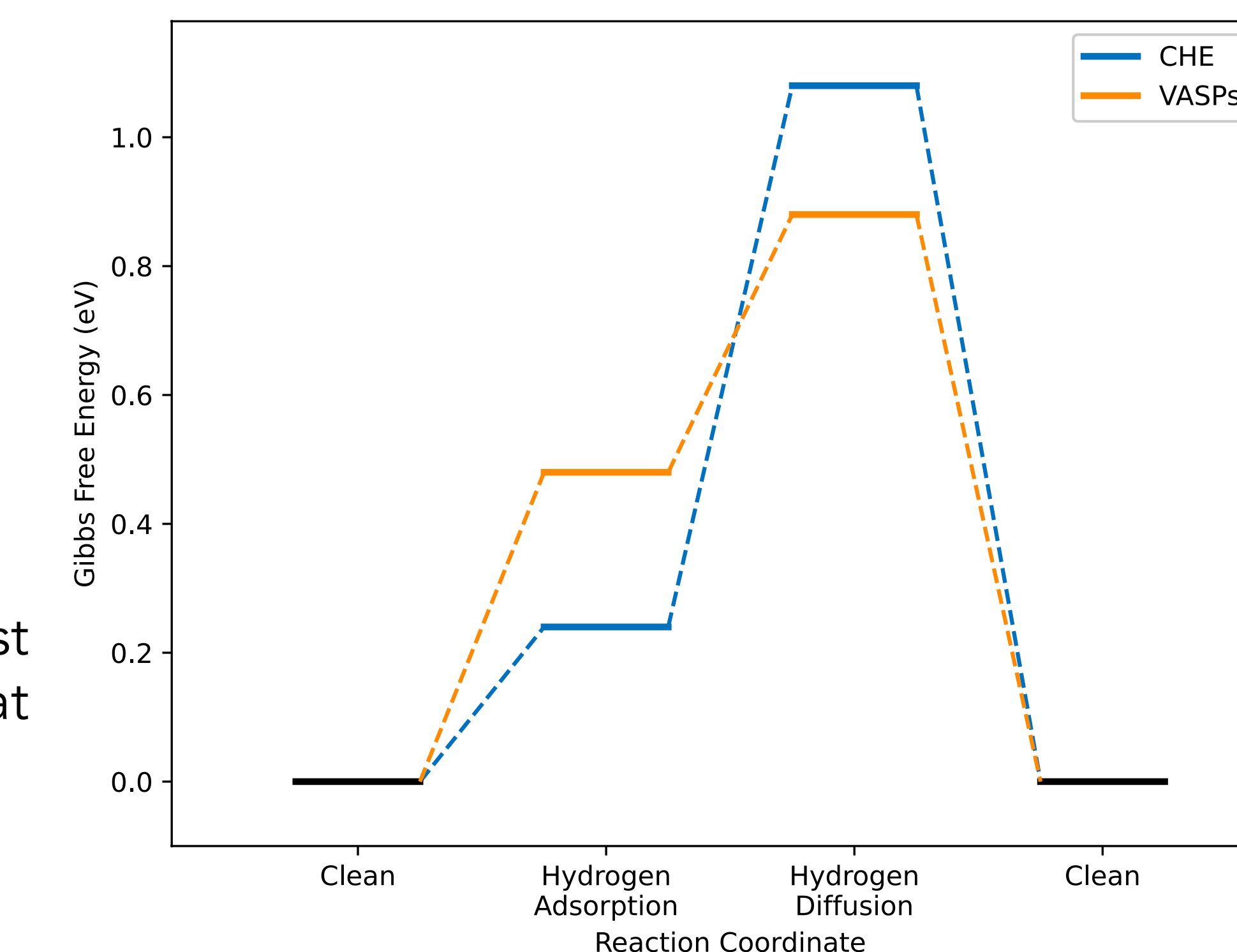
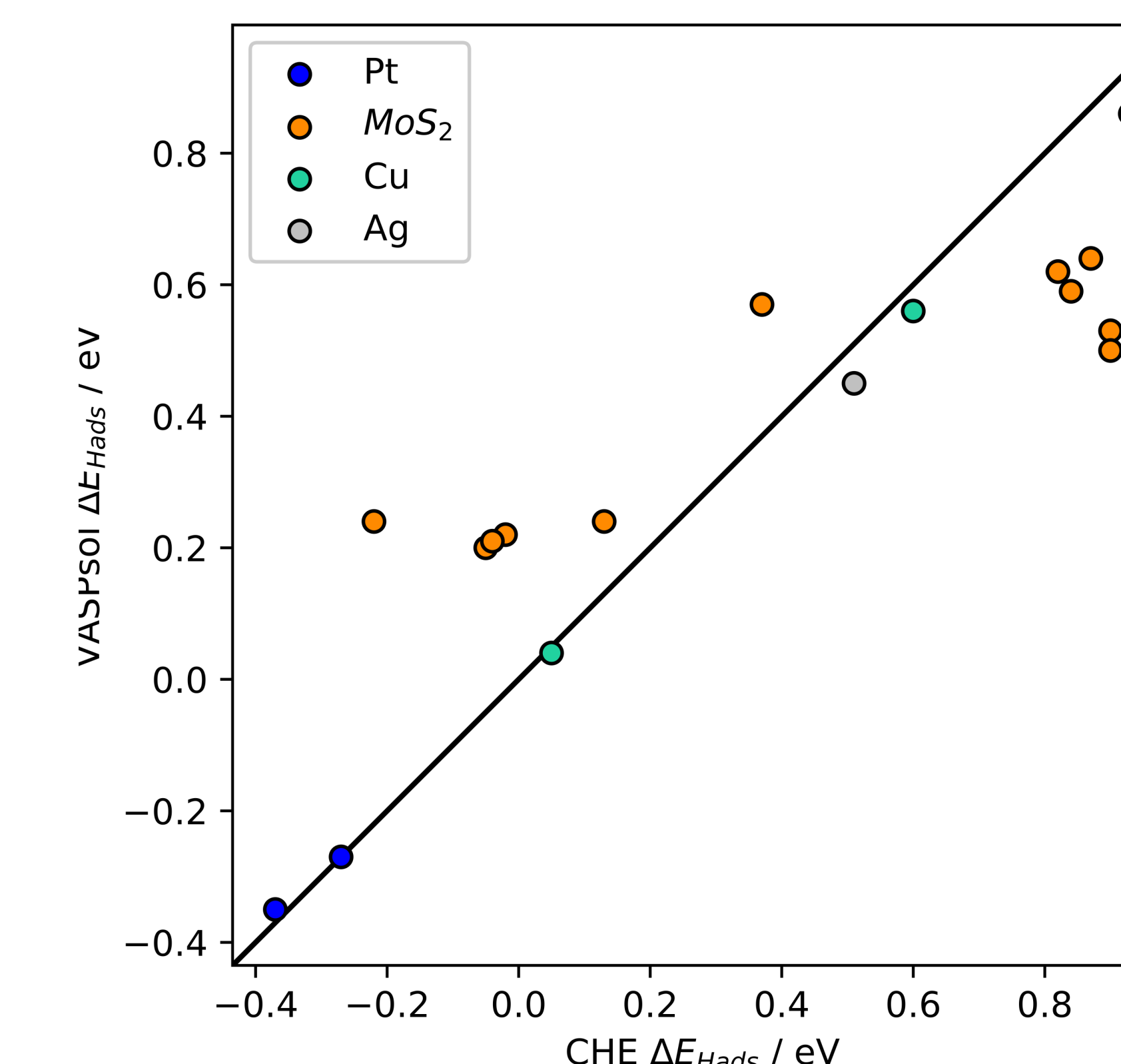
How do We Model the Potential of the System?

The computational hydrogen electrode (CHE), developed by Nørskov *et al.*² solves the first problem. The energy of the electrons is directly scaled by the potential: $-n(eU)$. Where n is the number of electrons, e the elementary charge and U the target potential.



The Vienna *ab initio* Simulation Package with the solvent module (VASPsol), developed by Mathew *et al.*³ solves both problems by including a background solvent layer with the capacity to model charge and therefore a double layer.

Comparing the Old with the New



Here we compare the difference between the two models in Gibbs free energies of a thermodynamic pathway for the HER (see left). Assuming the kinetic barriers are unaffected by the different models, the 0.2 eV difference we've calculated corresponds to an increase in the catalytic activity by 3 orders of magnitude.