Project 1: Grand Canonical Monte Carlo Simulations of Competitive Adsorption

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Relevant Files:

- The code implementing the algorithm and plotting (based on the provided pseudocode) is in **`MC_code.py`**.
- The code for running the example and reproducing the image from the project description is in **`run_example.py`**.
- The code for executing all scenarios and saving the figures is in **`run_project.py`**.
- All figures referenced in this document are located in the **`figures/`** folder.

Example Run to test code

After executing the example code, I obtained Figure 1, which closely resembles the image included in the project description. This confirms that the code functions correctly. (Note: The image is not properly formatted, as it is intended solely for verification purposes.)

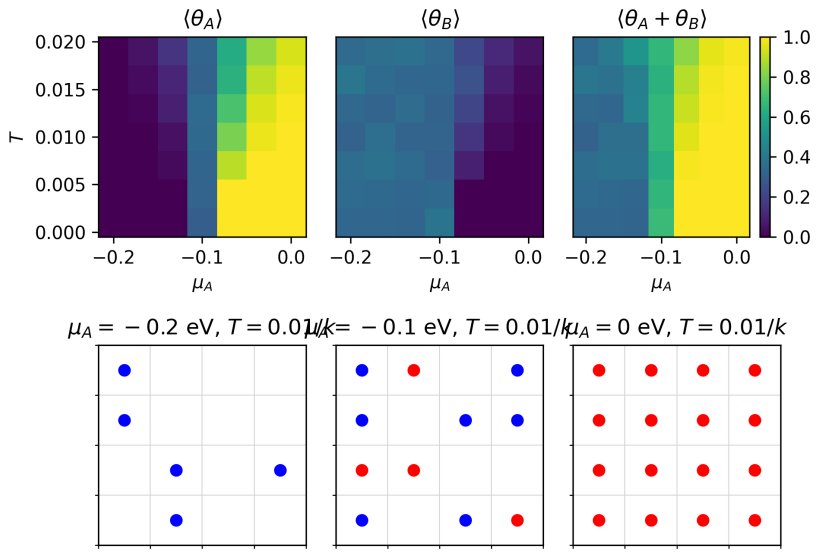

Figure 1: Output from the example run, replicating the reference image provided in the project description. This confirms the correct implementation of the algorithm.

Competitive absorption of H and N for ammonia synthesis

All five scenarios were executed, and representative phase diagrams are plotted below. The temperature is expressed in dimensionless units, while the chemical potentials are given in electron volts (eV). Surface coverages are represented as fractions between 0 and 1, where 1 indicates full coverage.

Scenario 1:

Ideal Mixture of Nitrogen and Hydrogen

Conditions: $\epsilon_N = -0.1\ eV, \epsilon_H = -0.1\ eV, \epsilon_{NN} = 0\ eV, \epsilon_{HH} = 0\ eV, \epsilon_{NH} = 0\ eV$

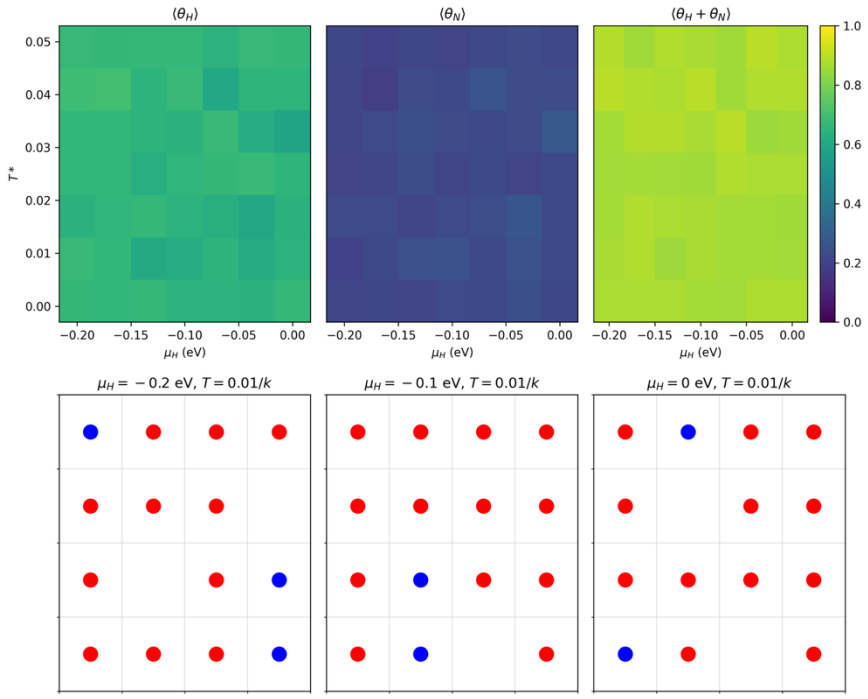

Figure 2: Phase diagram showing complete hydrogen coverage with minimal nitrogen presence, driven by entropy, for the ideal mixing condition.

Random mixing implies that there are no preferred bonding types. Consequently, the molecular coverage depends on the availability of hydrogen and nitrogen.

In **Figure 2**, there is complete hydrogen coverage with only a few nitrogen particles, a distribution dictated by entropy (modeled using Boltzmann probability). In this scenario, very few N–H bonds are formed, making it an unrealistic condition. Therefore, ammonia formation is unlikely at high hydrogen concentrations.

Scenario 2:

Repulsive Interactions between Nitrogen and Hydrogen

Conditions: $\epsilon_N = -0.1\ eV, \epsilon_H = -0.1\ eV, \epsilon_{NN} = 0.05\ eV, \epsilon_{HH} = 0.05\ eV, \epsilon_{NH} = 0.05\ eV$

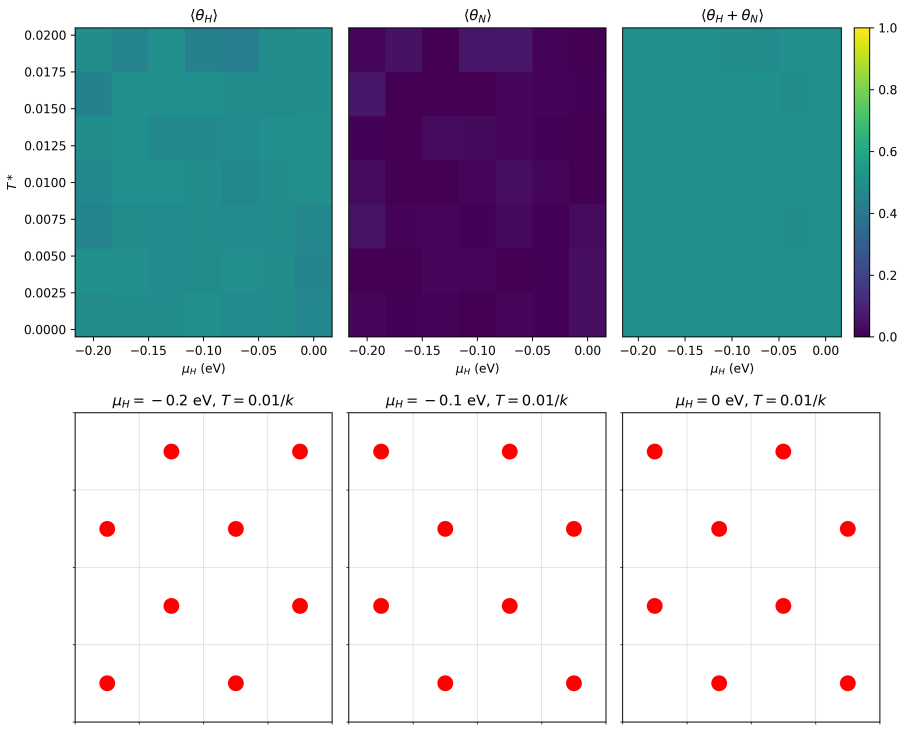

Figure 3: Phase diagram illustrating a scenario with partial hydrogen coverage (~0.5) and no nitrogen atoms for the "all repulsion" condition.

In this scenario, none of the components exhibit mutual affinity. Many empty sites remain because hydrogen atoms tend to avoid sitting next to each other. Although the hydrogen coverage is relatively high (around 0.5), there are no nitrogen atoms present to form ammonia. Therefore, this condition is also not useful for ammonia synthesis.

Scenario 3:

Attractive Interactions between Nitrogen and Hydrogen

Conditions:$\epsilon_N = -0.1\ eV, \epsilon_H = -0.1\ eV, \epsilon_{NN} = -0.05\ eV, \epsilon_{HH} = -0.05\ eV, \epsilon_{NH} = -0.05\ eV$

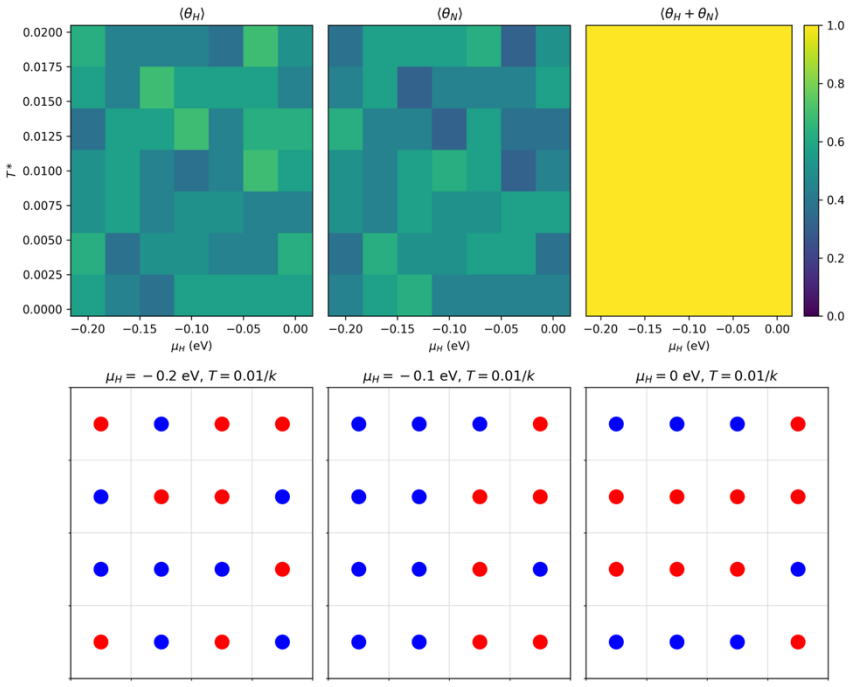

Figure 4: Phase diagram showing favorable interactions between nitrogen and hydrogen, leading to balanced coverage, illustrating the "All Attraction" condition.

In this scenario, all interactions are favorable, resulting in good coverage of both nitrogen and hydrogen across most chemical potentials and temperatures. However, at higher hydrogen chemical potentials, increased hydrogen absorption reduces the formation of N–H bonds, which may lower ammonia concentrations. Additionally, since all bonds are favorable, ammonia molecules may not desorb easily. Therefore, this condition is most favorable for ammonia synthesis at lower hydrogen chemical potentials.

Scenario 4:

Immiscible Nitrogen and Hydrogen

Conditions: $\epsilon_N = -0.1\ eV, \epsilon_H = -0.1\ eV, \epsilon_{NN} = -0.05\ eV, \epsilon_{HH} = -0.05\ eV, \epsilon_{NH} = 0.05\ eV$

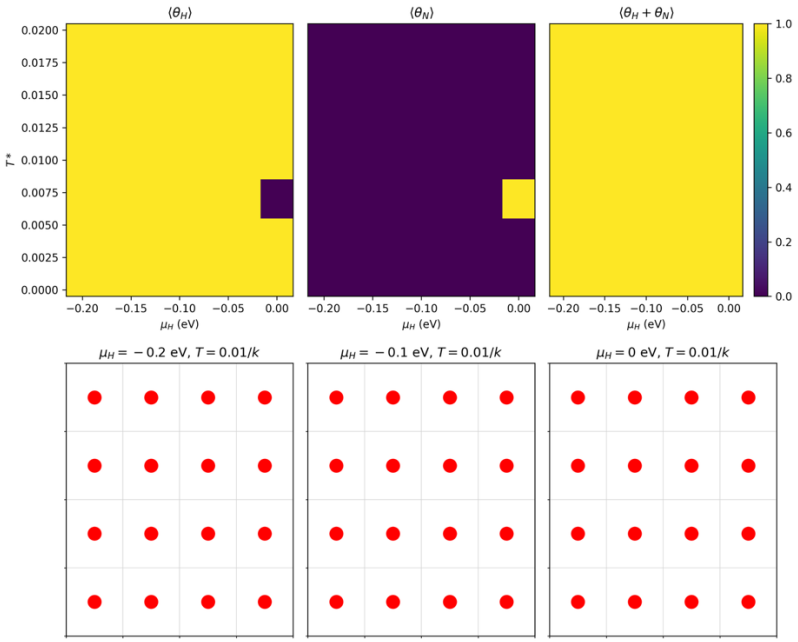

Figure 5: Phase diagram illustrating segregation of nitrogen and hydrogen into separate clusters. This condition does not promote N–H bond formation, making it unsuitable for ammonia synthesis.

In this scenario, nitrogen and hydrogen tend to segregate, as shown in the figure by clusters of hydrogen atoms (larger sizes) and likely nitrogen clusters forming as well. By definition, this condition does not favor N–H bond formation and is therefore not useful for ammonia synthesis.

Scenario 5:

Like Dissolves Unlike

Conditions: $\epsilon_N = -0.1\ eV, \epsilon_H = -0.1\ eV, \epsilon_{NN} = 0.05\ eV, \epsilon_{HH} = 0.05\ eV, \epsilon_{NH} = -0.05\ eV$

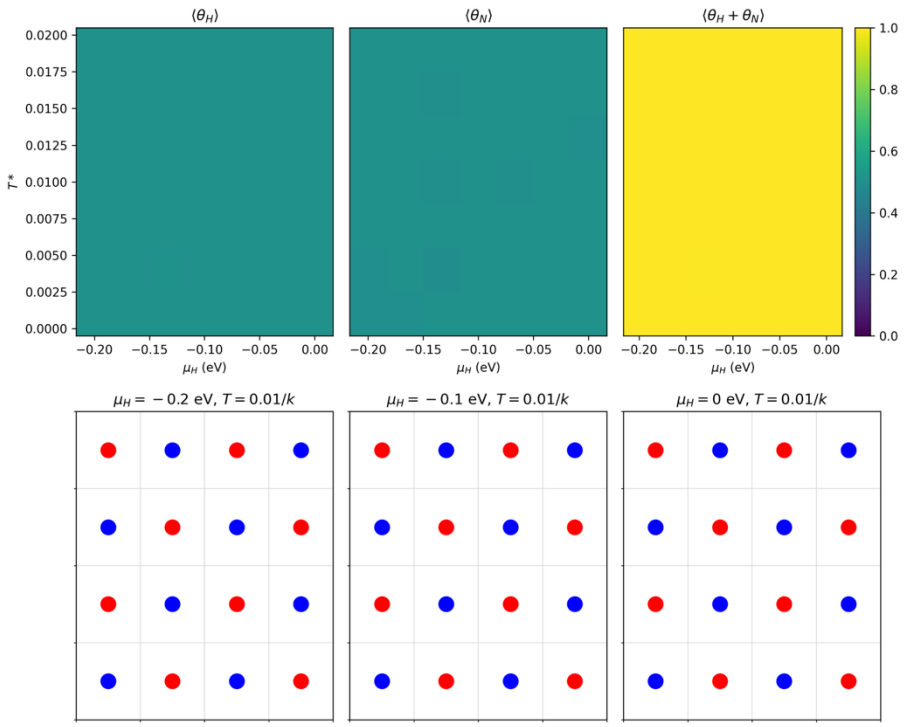

Figure 6: Ordered configuration maximizing N–H bonds and coverage, illustration "Like dissolves unlike" condition.

In this scenario, an ordered configuration is formed, maximizing N–H bonds and achieving near-complete coverage, making it the ideal condition for ammonia synthesis. However, at higher temperatures, disorder becomes more favorable, and the system tends toward an ideal lattice configuration. At room temperature and slightly elevated temperatures, this condition ensures maximum N–H bonding.

In conclusion, the *"**Like Dissolves Unlike**"* scenario provides the most favorable conditions for ammonia synthesis, while the *"**All Bonds Attractive**"* scenario is also a reasonable option for obtaining ammonia production.
