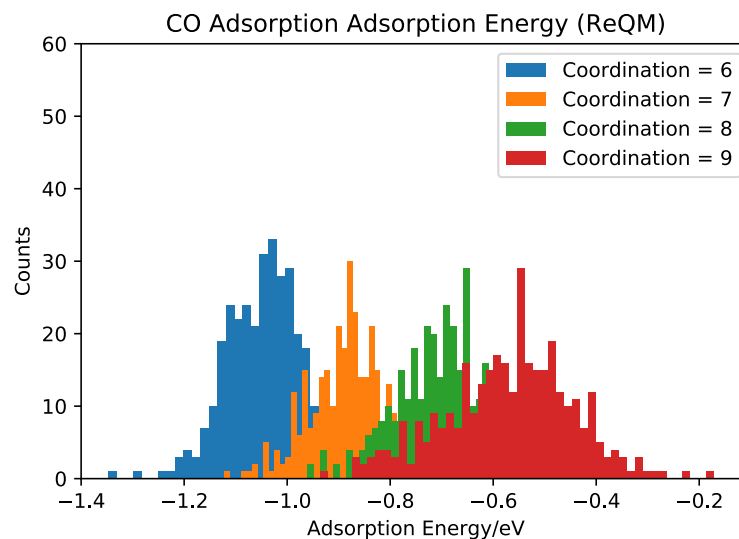
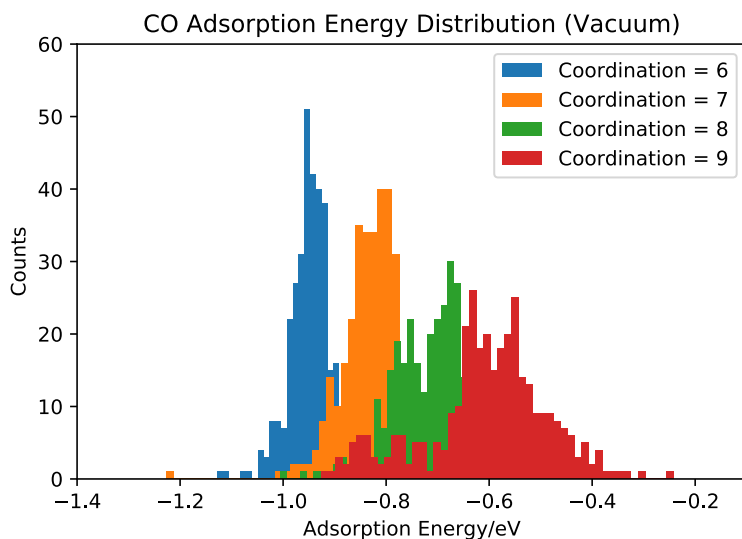
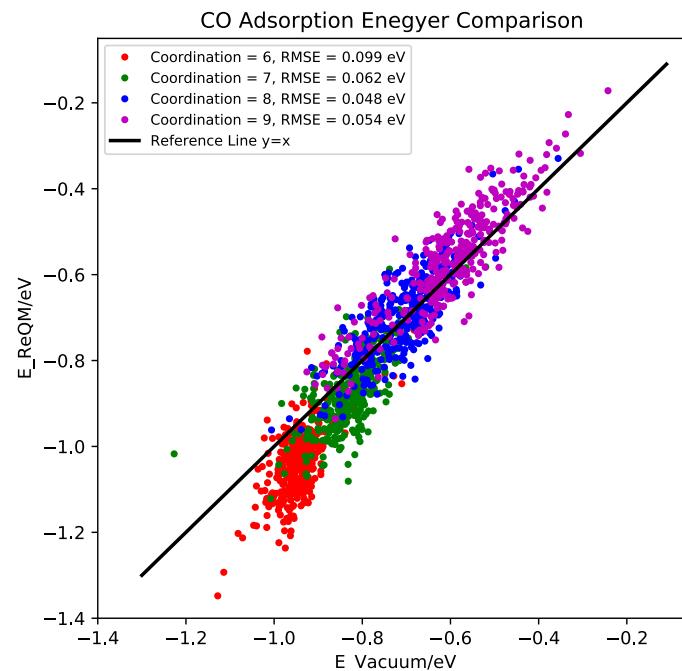
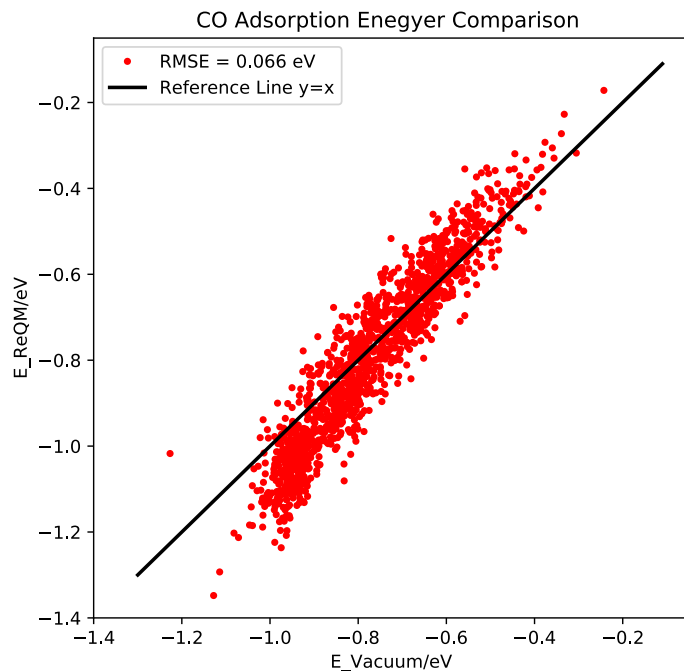
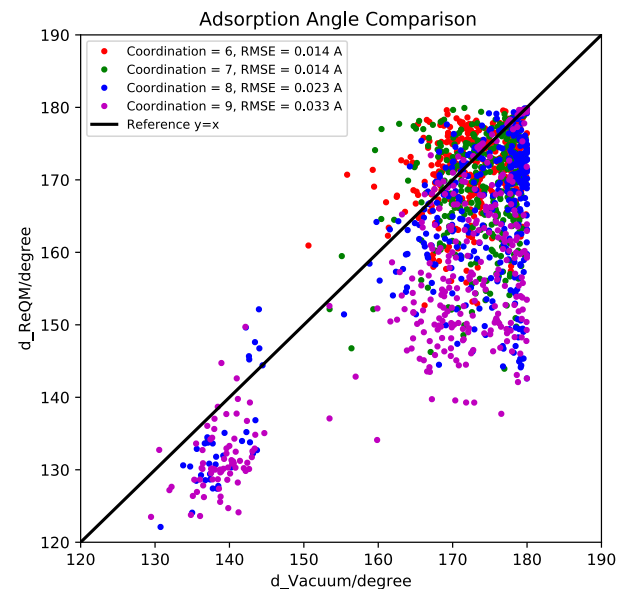
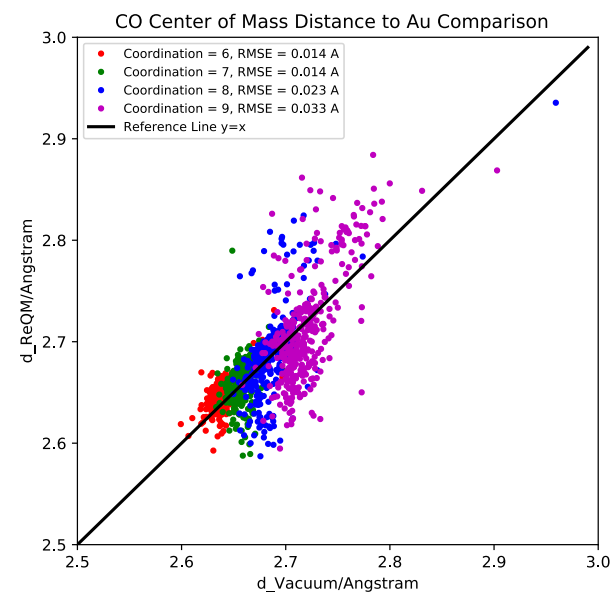
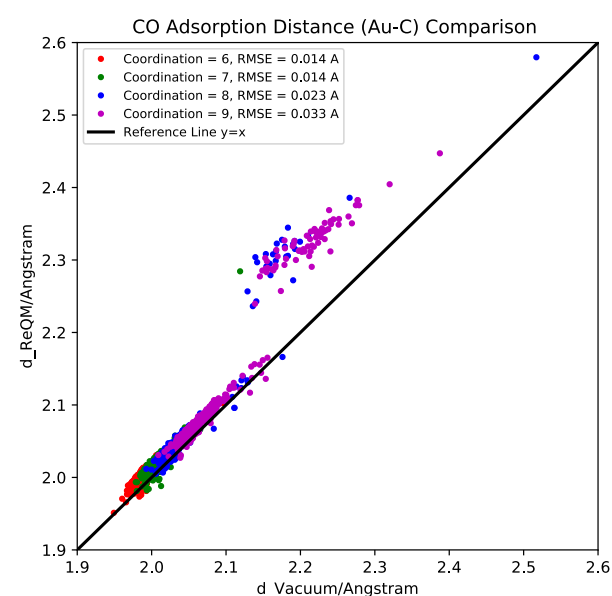
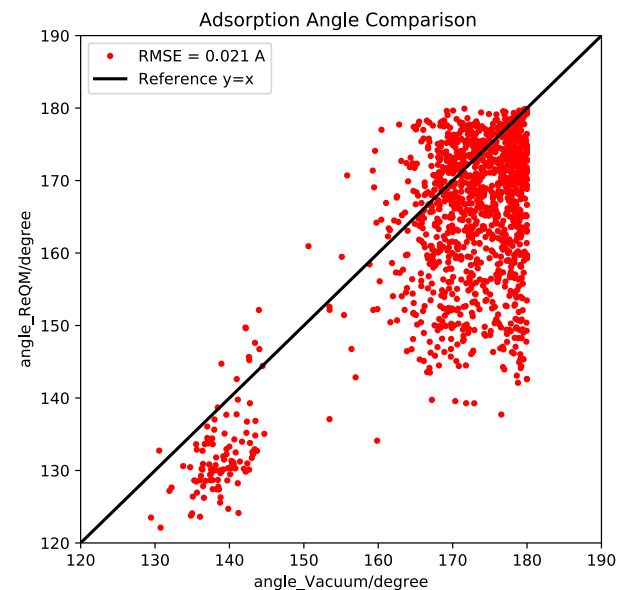
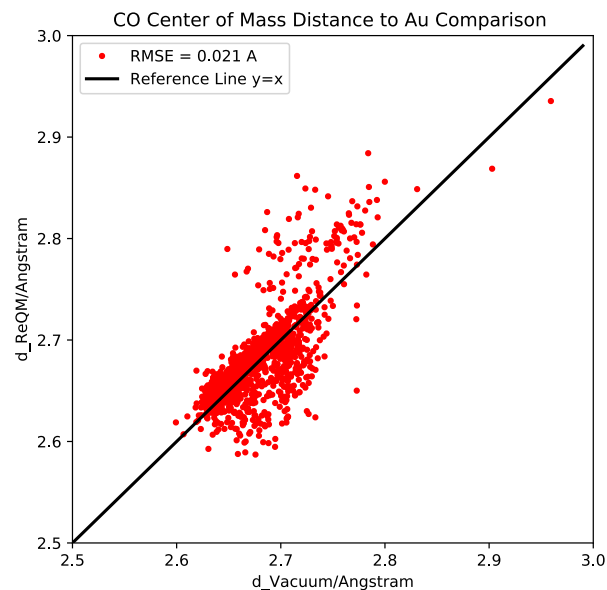
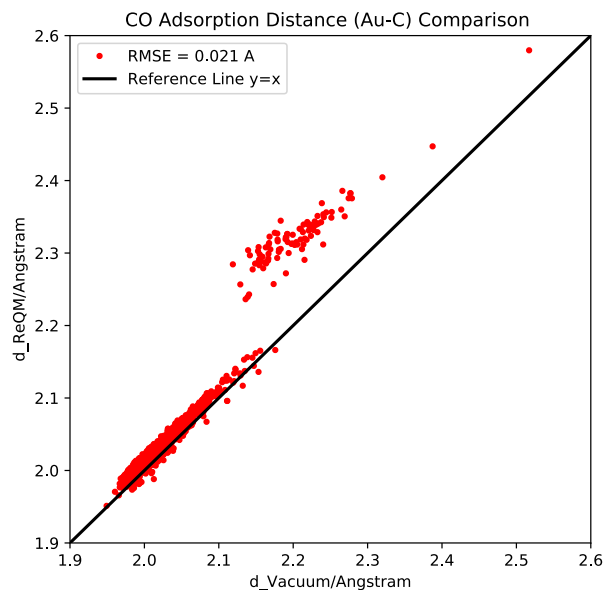


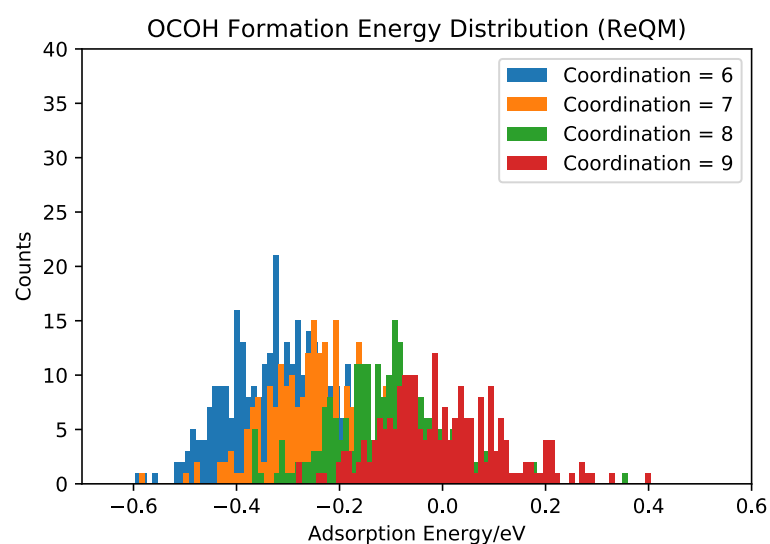
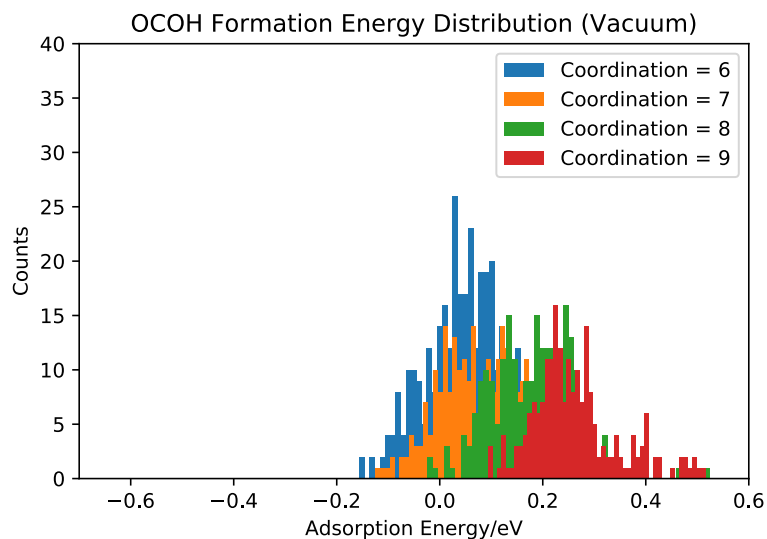
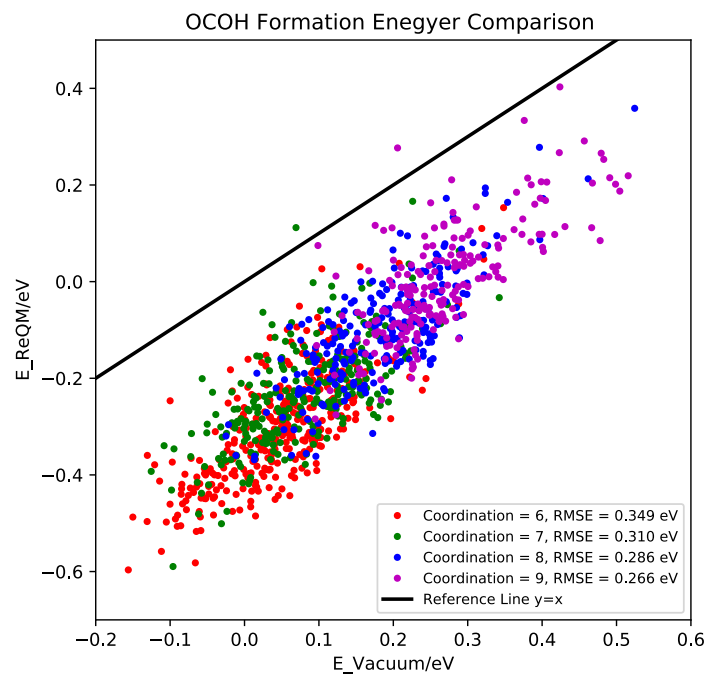
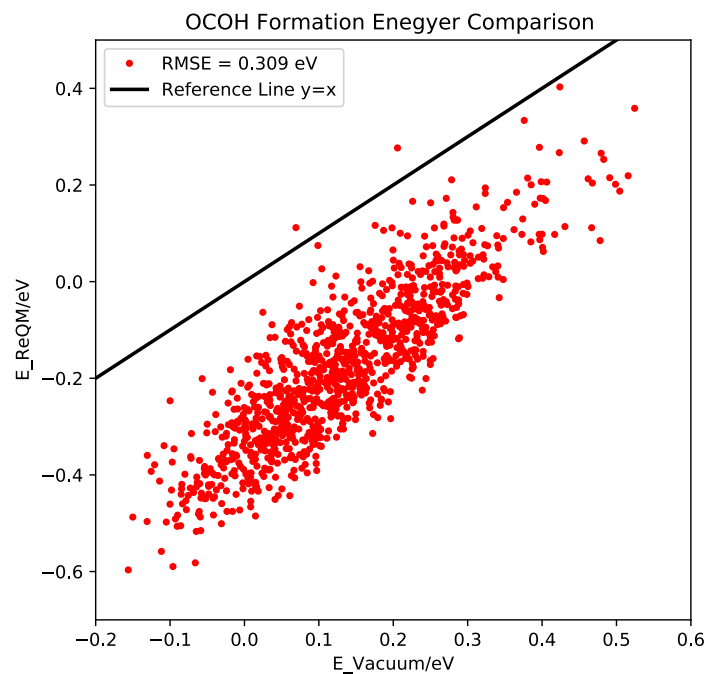
Comparison of CO Adsorption Energy: ReQM vs Vacuum



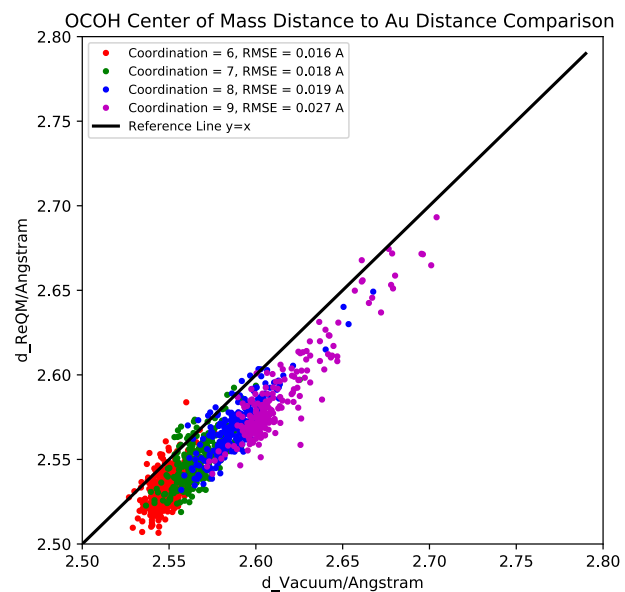
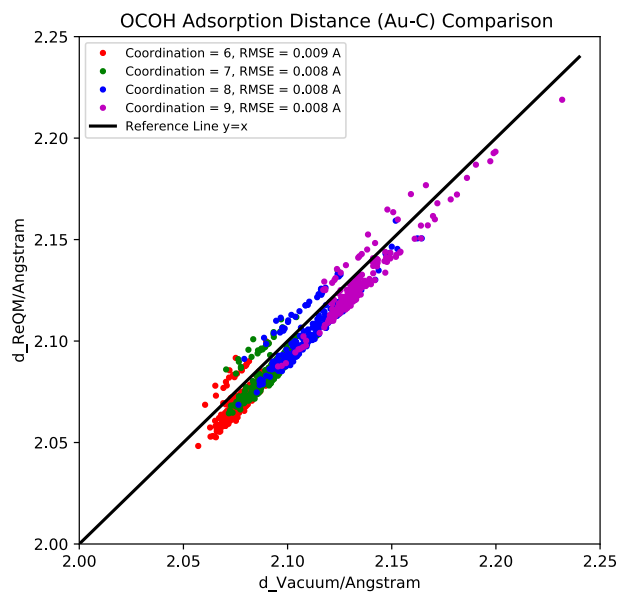
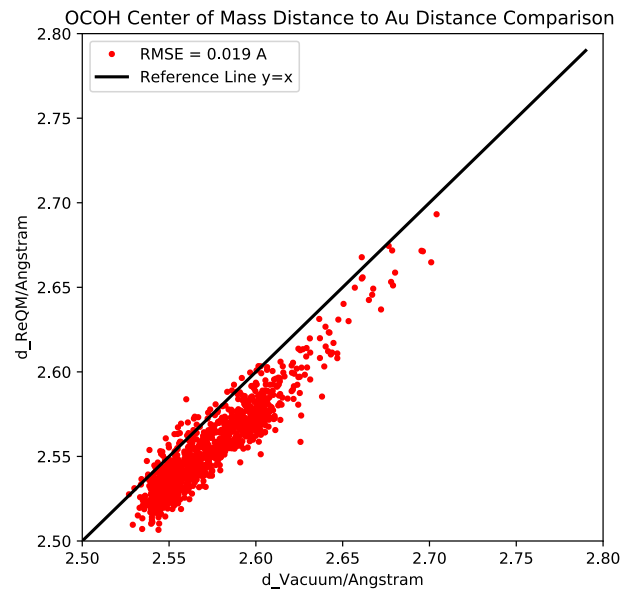
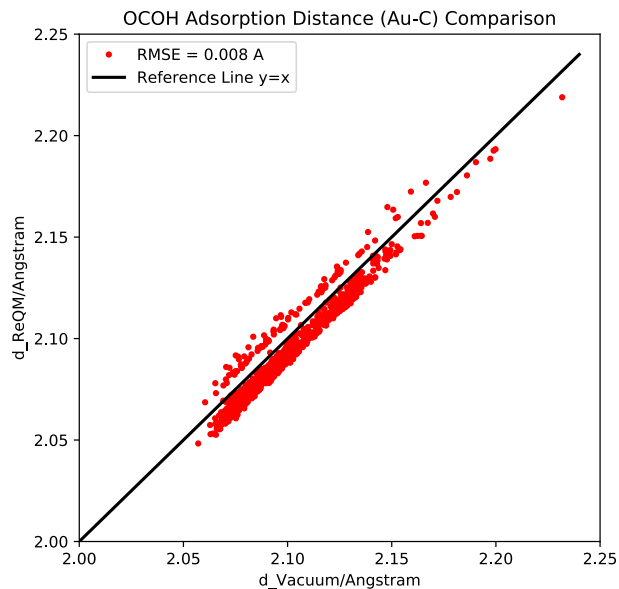
Comparison of CO Adsorption Conformation: ReQM vs Vacuum



Comparison of OCOH Formation Energy: ReQM vs Vacuum



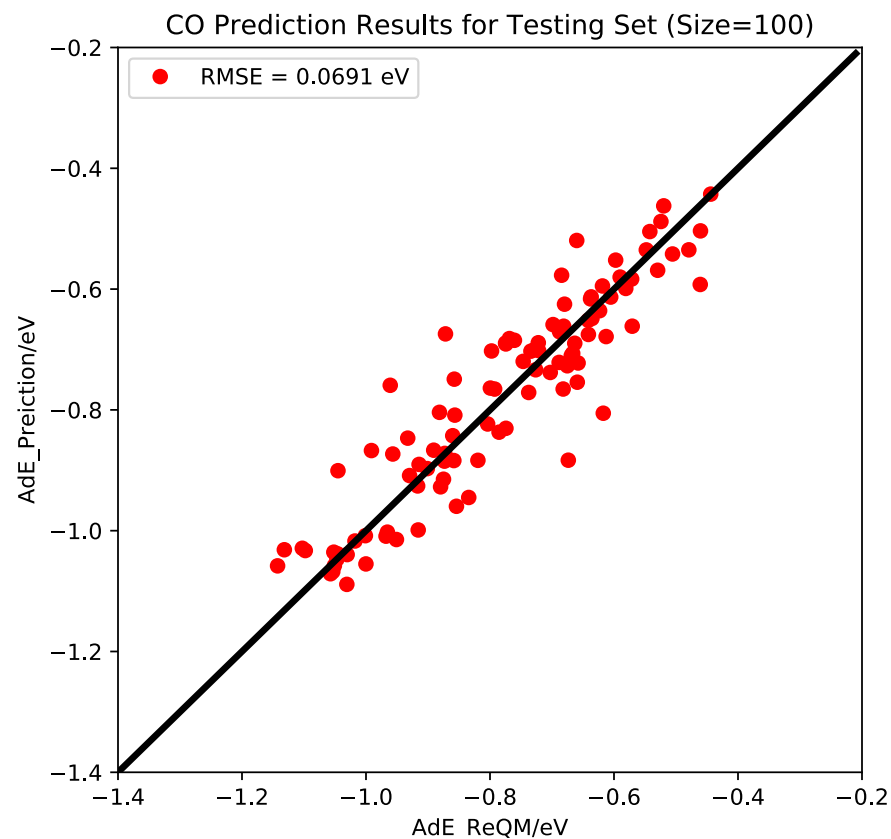
Comparison of OCOH Conformation: ReQM vs Vacuum



CO Adsorption Energy Training Results

| Training Size | Training RMSE/eV | Validation RMSE/eV | Test RMSE/eV |
|---------------|------------------|--------------------|---------------|
| 200 | 0.0692 | 0.0913 | 0.0780 |
| 400 | 0.0703 | 0.0840 | 0.0789 |
| 600 | 0.0704 | 0.0814 | 0.0732 |
| 800 | 0.0719 | 0.0782 | 0.0720 |
| <u>1184</u> | <u>0.0748</u> | <u>0.0758</u> | <u>0.0691</u> |

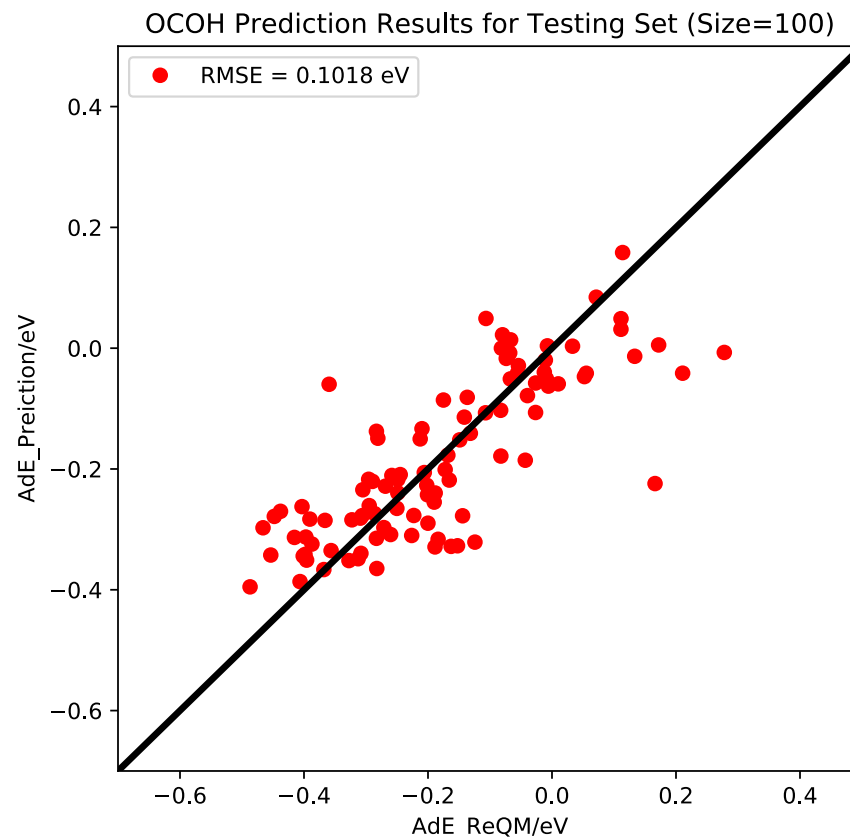
Final Training: 1184 in Training Set
100 in Validation Set
100 in Test Set



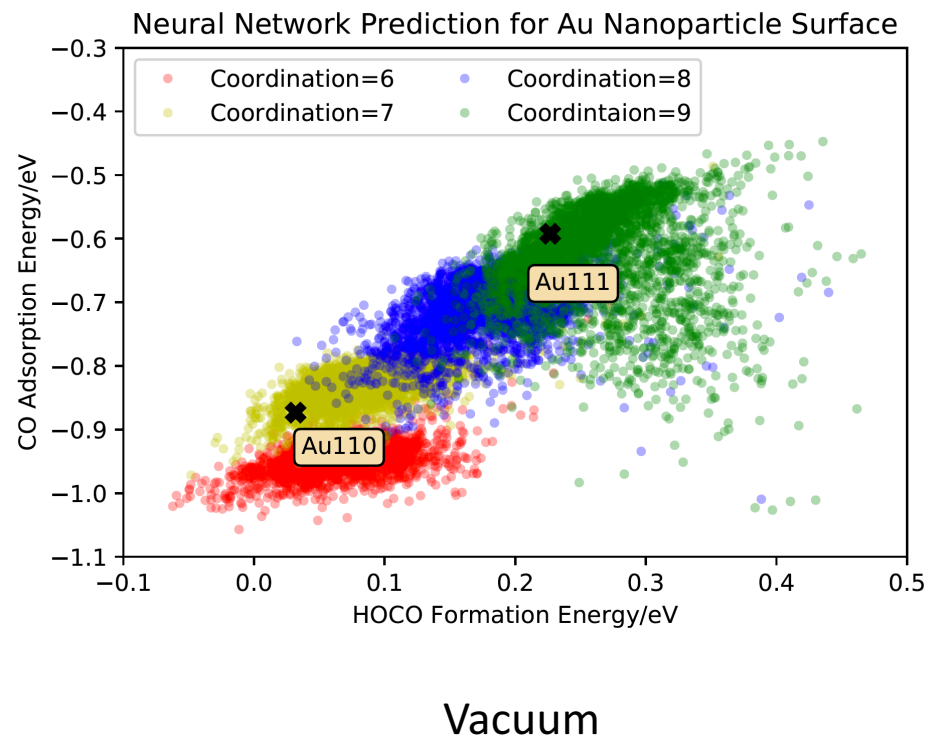
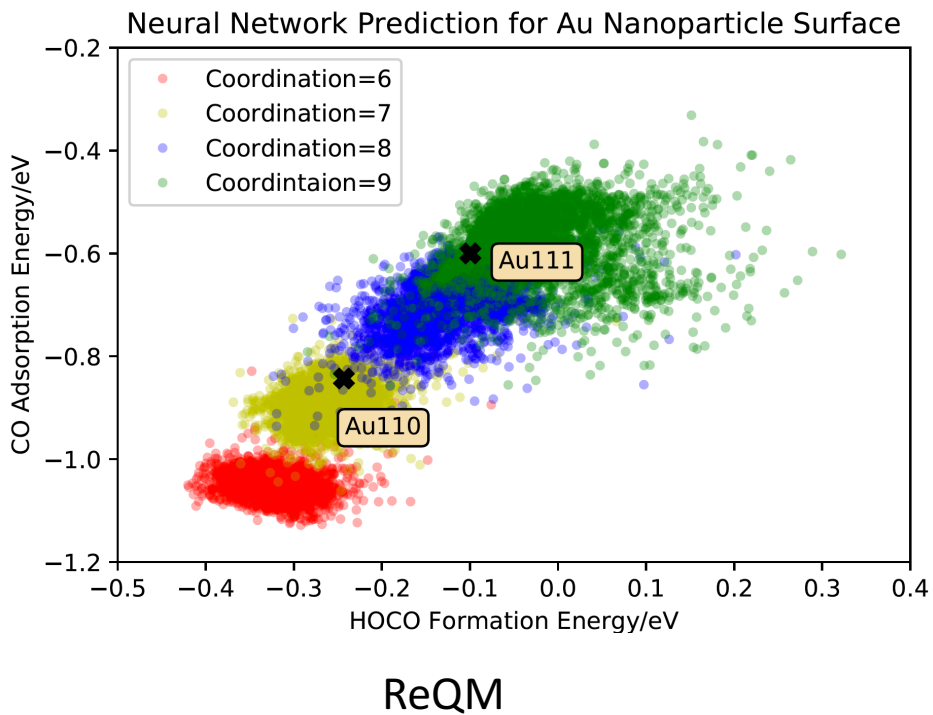
OCOH Formation Energy Training Results

| Training Size | Training RMSE/eV | Validation RMSE/eV | Test RMSE/eV |
|---------------|------------------|--------------------|---------------|
| 200 | 0.0908 | 0.1033 | 0.1178 |
| 400 | 0.0896 | 0.1027 | 0.1081 |
| 600 | 0.0920 | 0.1002 | 0.1027 |
| 800 | 0.0923 | 0.0985 | 0.1026 |
| <u>859</u> | <u>0.0928</u> | <u>0.0969</u> | <u>0.1017</u> |

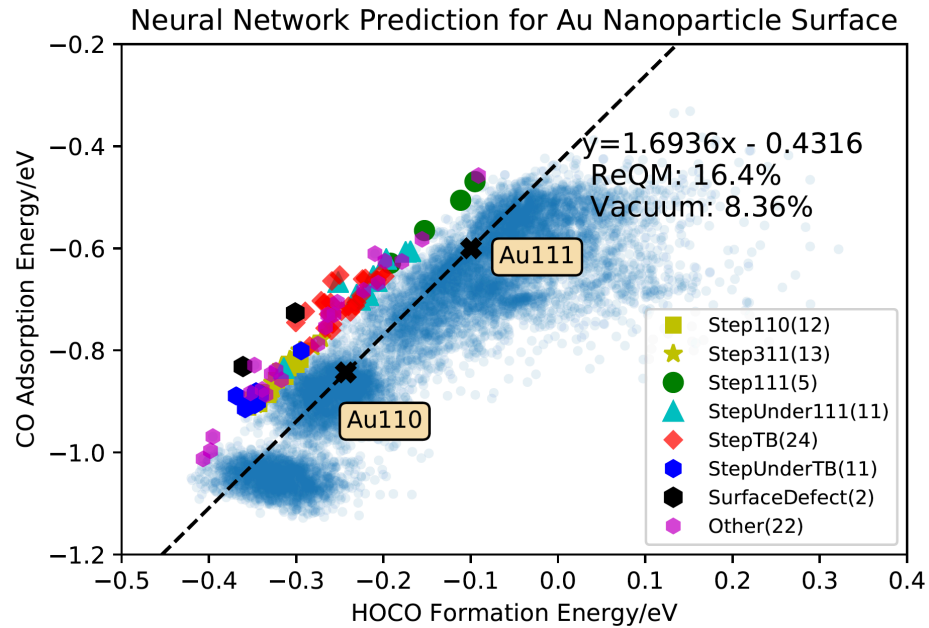
Final Training: 859 in Training Set
100 in Validation Set
100 in Test Set



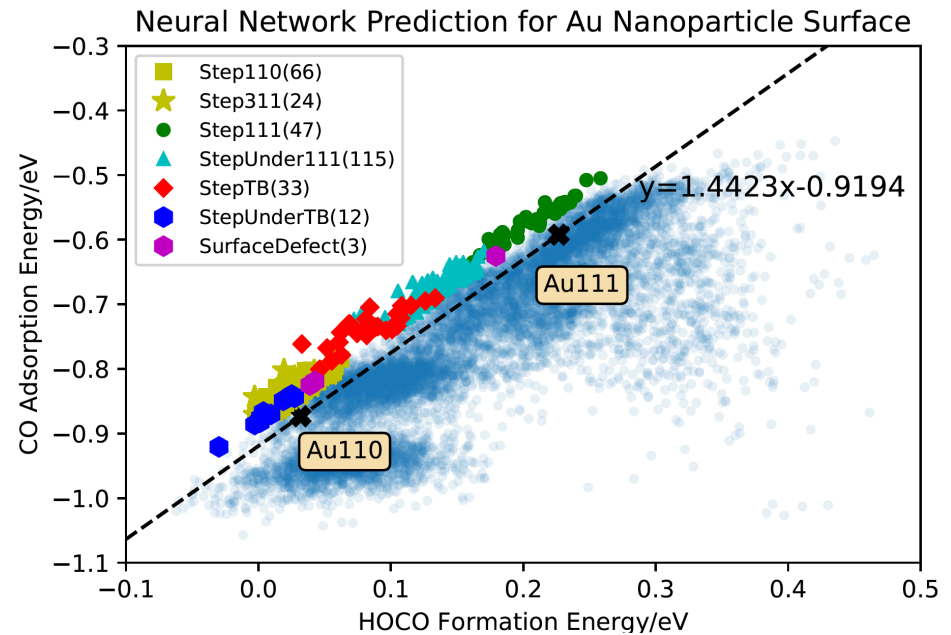
Prediction on AuNP Surface



Prediction on AuNP Surface



ReQM

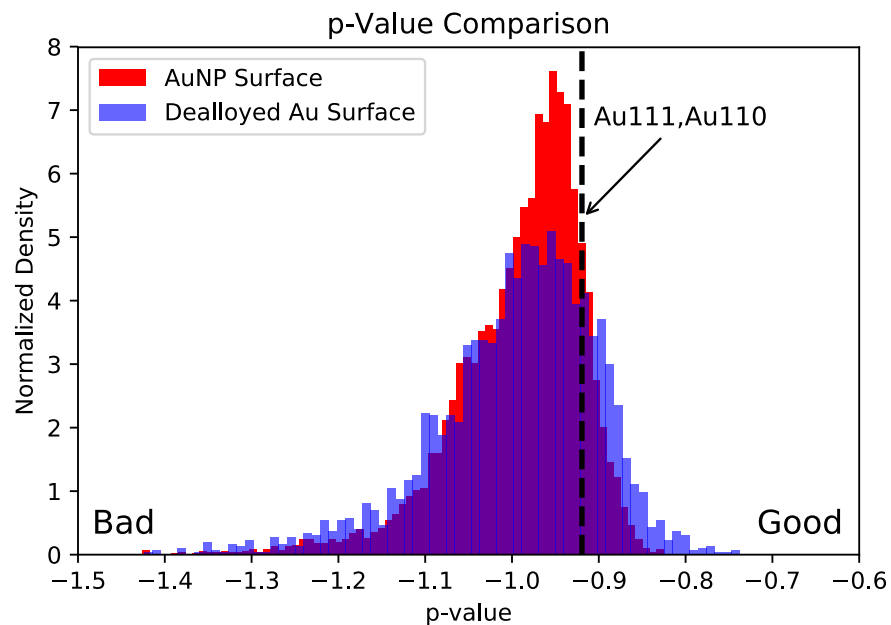
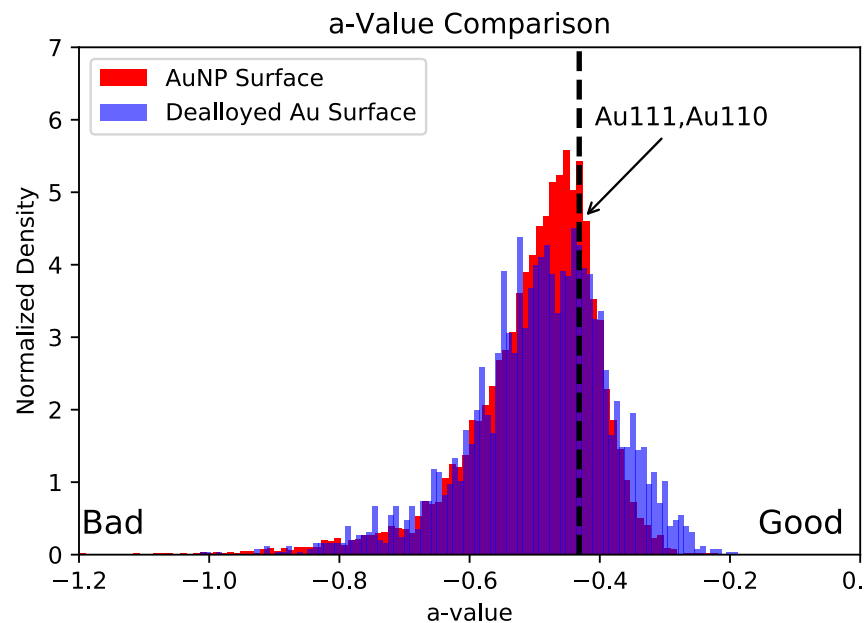


Vacuum

Sites Ratio above the line defined by Au111 and Au110:

- ReQM: 16.4 %
- Vacuum: 8.36 %

AuNP vs Dealloyed Au Surface



$$AR = \frac{\text{number of sites with } a > -0.4194}{\text{total number of surface sites}}$$

| AR | AuNP | De-alloyed Au |
|--------|--------|---------------|
| ReQM | 0.1640 | 0.1831 |
| Vacuum | 0.0836 | 0.1370 |