# Supplementary Information: Benchmarking Machine-Learned Potentials for Adsorption on Pt and $IrO_2$ Surfaces Using OC20 and OMat24

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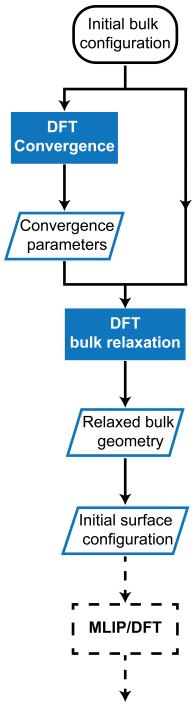


**Figure S1:** Both Pt and $IrO_2$ slab bulk configurations were relaxed using DFT; the lattice parameter of the resulting relaxed bulk geometry was used to design subsequent surface configurations for adsorption calculations

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**Table S1:** The adsorption energies of common adsorbates like CO, NO, O, and H on Pt(111) and Pt(110) calculated using UMA-OC20, obtained from experiments (Silbaugh and Campbell), and computed using spin-polarized DFT without vdW corrections. Here, both the DFT flavors and the geometries are different

| Surface | Adsorbate | Coverage | UMA-OC20 | | Exp. | Diff. | DFT | | Diff. OC20-DFT | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | $E_{ads}$ (eV) | Site | $E_{ads}$ (eV) | OC20-Exp. (eV) | $E_{ads}$ (eV) | Site | $E_{ads}$ (eV) | Norm (Å) |
| Pt (111) | CO | 1/4 | -1.493 | fcc | -1.244 | -0.249 | -1.420 | fcc | -0.073 | 0.085 |
| | NO | 1/4 | -1.741 | bridge, fcc | -1.182 | -0.559 | -1.538 | fcc | -0.203 | 0.094 |
| | $O_2 \rightarrow$ 2O | 1/9 | -3.092 | fcc | -2.156 | -0.936 | -2.025 | fcc | -1.067* | 0.179 |
| | $H_2 \rightarrow$ 2H | 1/4 | -0.681 | fcc | -0.746 | 0.065 | -0.718 | top** | 0.037 | 0.066 |
| Pt (110) | CO | 1/4 | -1.858 | short bridge | -1.244 | -0.614 | -1.829 | short bridge | -0.029 | 0.074 |
| | NO | 1/4 | -2.290 | short bridge | -1.171 | -1.119 | -2.039 | short bridge | -0.251 | 0.102 |
| | $O_2 \rightarrow$ 2O | 1/4 | -3.412 | short bridge | -2.28 | -1.132 | -2.174 | short bridge | -1.238* | 0.113 |

*Gas phase references, $E_{gas}$, for each adsorbate was computed as a linear combination of $N_2$, $H_2O$, CO, and $H_2$ resulting in the atomic energies of $O_2$ to be -14.408 eV (correct value from DFT is -10.545)

** The fcc site is shown to be the most stable site for *H on Pt(111). Adding vdW corrections to DFT changes the site from top to fcc.

**Table S2:** The adsorption energies of common adsorbates like CO, NO, O, and H on Pt(111) and Pt(110) calculated from MLIPs UMA-OC20 and non-spin polarized DFT with no vdW corrections. Here, the DFT flavors are the same but the geometries are different

| Surface | Adsorbate | Coverage | UMA-OC20 | | DFT | | Diff. OC20-DFT | |
|---|---|---|---|---|---|---|---|---|
| | | | $E_{ads}$ (eV) | Site | $E_{ads}$ (eV) | Site | $E_{ads}$ (eV) | Norm (Å) |
| Pt(111) | CO | 1/4 | -1.493 | fcc | -1.420 | fcc | -0.073 | 0.085 |
| | NO | 1/4 | -1.741 | bridge, fcc | -1.844 | fcc | 0.103 | 0.094 |
| | $O_2 \rightarrow$ 2O | 1/9 | -3.092 | fcc | -3.050 | fcc | -0.042 | 0.158 |
| | $H_2 \rightarrow$ 2H | 1/4 | -0.646 | top* | -0.718 | top* | 0.072 | 0.066 |
| Pt(110) | CO | 1/4 | -1.858 | short bridge | -1.829 | short bridge | -0.029 | 0.074 |
| | NO | 1/4 | -2.290 | short bridge | -2.338 | short bridge | 0.048 | 0.08 |
| | $O_2 \rightarrow$ 2O | 1/4 | -3.412 | short bridge | -3.298 | short bridge | -0.114 | 0.106 |

**Table S3:** The adsorption energies of common adsorbates like CO, NO, O, and H on Pt(111) and Pt(110) calculated from single-point MLIPs UMA-OC20 and non-spin polarized DFT with no vdW corrections, on the relaxed structure obtained from the non-spin polarized DFT with no vdW corrections. Here, both the DFT flavors and the geometries are the same. All Euclidean Norm of coordinate difference is 0 and hence, is not displayed

| Surface | Adsorbate | Coverage | UMA-OC20 | | DFT | | Diff. |
|---|---|---|---|---|---|---|---|
| | | | $E_{ads}$ (eV) | Site | $E_{ads}$ (eV) | Site | OC20-DFT (eV) |
| Pt(111) | CO | 1/4 | -1.490 | fcc | -1.420 | fcc | -0.070 |
| | NO | 1/4 | -1.739 | bridge, fcc | -1.844 | fcc | 0.105 |
| | $O_2 \rightarrow$ 2O | 1/9 | -3.070 | fcc | -3.050 | fcc | -0.020 |
| | $H_2 \rightarrow$ 2H | 1/4 | -0.644 | top* | -0.718 | top* | 0.074 |
| Pt(110) | CO | 1/4 | -1.866 | shortbridge | -1.829 | shortbridge | -0.037 |
| | NO | 1/4 | -2.299 | shortbridge | -2.338 | shortbridge | 0.039 |
| | $O_2 \rightarrow$ 2O | 1/4 | -3.414 | shortbridge | -3.298 | shortbridge | -0.116 |

**Table S4:** The adsorption energies of common adsorbates like CO, NO, O, and H on Pt(231) calculated from single-point MLIPs UMA-OC20 and non-spin polarized DFT with no vdW corrections, on structures with the adsorbate 2 Å from three top sites corresponding to the three Pt atoms exposed to vacuum. Here, both the DFT flavors and the geometries are the same. All Norm is 0 and hence, is not displayed

| Surface | Adsorbate | Coverage | Site | $E_{ads}$ | | Diff. |
|---|---|---|---|---|---|---|
| | | | | UMA-OC20 (eV) | DFT (eV) | OC20-DFT (eV) |
| Pt(231) | CO | 1/4 | site1 | -1.782 | -1.669 | -0.113 |
| | | | site2 | 0.149 | 0.210 | -0.061 |
| | | | site3 | -0.060 | -0.007 | -0.053 |
| | NO | 1/4 | site1 | -1.794 | -1.842 | 0.048 |
| | | | site2 | -0.261 | -0.339 | 0.078 |
| | | | site3 | -0.664 | -0.726 | 0.062 |
| | O | 1/4 | site1 | -0.575 | -0.470 | -0.105 |
| | | | site2 | 2.265 | 2.278 | -0.013 |
| | | | site3 | 2.147 | 2.123 | 0.024 |
| | H | 1/4 | site1 | 0.498 | 0.546 | -0.048 |
| | | | site2 | 2.249 | 2.244 | 0.005 |
| | | | site3 | 2.162 | 2.185 | -0.023 |

**Table S5:** The adsorption energies of *NO and *O on Pt(111) and Pt(110) calculated from spin polarized and non-spin polarized DFT, along with MLIP

| Technique | Spin state | Slab | Adsorbate (X) | $E_{ads}$(X) (eV) | E(slab+*X) (eV) | E(slab) (eV) | $E(X_{ref\ gas})$ (eV) |
|---|---|---|---|---|---|---|---|
| DFT | Spin | Pt(111)- 2×2 | NO | -1.538 | -126.287 | -111.864 | -12.885 |
| | No spin | | | -1.844 | -126.287 | -111.864 | -12.579 |
| MLIP | | | | -1.741 | -118.118 | -104.675 | -11.702 |
| DFT | Spin | Pt(111)- 3×3 | O* | -1.013 | -257.926 | -251.641 | -5.273 |
| | No spin | | | -1.525 | -257.871 | -251.641 | -4.705 |
| MLIP | | | | -1.546 | -241.301 | -235.519 | -4.236 |
| DFT | Spin | Pt(110)- 2×2 | NO | -2.039 | -121.861 | -106.937 | -12.885 |
| | No spin | | | -2.338 | -121.855 | -106.937 | -12.579 |
| MLIP | | | | -2.290 | -113.617 | -99.625 | -11.702 |
| DFT | Spin | | O* | -1.087 | -113.297 | -106.937 | -5.273 |
| | No spin | | | -1.649 | -113.292 | -106.937 | -4.705 |
| MLIP | | | | -1.706 | -105.567 | -99.625 | -4.236 |

* The adsorption energy for O is for a coverage of 1 O in the slab, which is half of the value depicted in other tables which consider 2 O in the slab. The reference gas column for O depicts 0.5*E($O_2$ gas)

**Table S6:** The adsorption energies of *NO and *O on Pt(111) and Pt(110) calculated from spin polarized and non-spin polarized DFT. Most of the difference between them arise from the reference gas calculations. We obtain the same adsorption energies for *CO and *H on Pt(111) and Pt(110) from both spin-polarized and non-spin polarized DFT

| Spin state | Slab | Adsorbate (X) | $E_{ads}$(X) (eV) | E(slab+*X) (eV) | E(slab) (eV) | $E(X_{ref\ gas})$ (eV) | Norm Å |
|---|---|---|---|---|---|---|---|
| Spin | Pt(111)- 2×2 | NO | -1.538 | -126.287 | -111.864 | -12.885 | |
| No spin | | | -1.844 | -126.287 | -111.864 | -12.579 | |
| Difference | | | 0.306 | 0 | 0 | -0.306 | 0.022 |
| Spin | Pt(111)- 3×3 | O* | -1.013 | -257.926 | -251.641 | -5.273 | |
| No spin | | | -1.525 | -257.871 | -251.641 | -4.705 | |
| Difference | | | 0.512 | -0.055 | 0 | -0.567 | 0.046 |
| Spin | Pt(110)- 2×2 | NO | -2.039 | -121.861 | -106.937 | -12.885 | |
| No spin | | | -2.338 | -121.855 | -106.937 | -12.579 | |
| Difference | | | 0.3 | -0.006 | 0 | -0.306 | 0.044 |
| Spin | | O* | -1.087 | -113.297 | -106.937 | -5.273 | |
| No spin | | | -1.649 | -113.292 | -106.937 | -4.705 | |
| Difference | | | 0.562 | -0.006 | 0 | -0.567 | 0.021 |

* The adsorption energy for O is for a coverage of 1 O in the slab, which is half of the value depicted in other tables which consider 2 O in the slab. The reference gas column for O depicts 0.5*E($O_2$ gas)

**Table S7:** The adsorption energies of adsorbates in the water splitting reaction on $IrO_2(110)$ calculated from UMA-OMat24 MLIP and spin polarized DFT with vdW corrections. Here, the DFT flavors are the same. The SP and DFT geometries are the same but the rest are different from them

| Surface | Adsorbate | UMA-OMat24 $E_{ads}$ R1 (eV) | UMA-OMat24 $E_{ads}$ SP (eV) | UMA-OMat24 $E_{ads}$ R2 (eV) | DFT $E_{ads}$ (eV) | Difference R1-DFT $E_{ads}$ (eV) | Difference R1-DFT Norm (Å) | Difference SP-DFT $E_{ads}$ (eV) | Difference SP-DFT Norm (Å) | Difference R2-DFT $E_{ads}$ (eV) | Difference R2-DFT Norm (Å) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $IrO_2$ (110) | H, - | -0.848 | -1.809 | -1.819 | -1.746 | 0.898* | 9.125 | -0.063 | 0 | -0.073 | 0.244 |
| | H, H | -3.745 | -3.744 | -3.745 | -3.726 | -0.019 | 11.107 | -0.018 | 0 | -0.019 | 0.202 |
| | O, - | 2.383 | 2.427 | 2.383 | 2.491 | -0.108 | 6.817 | -0.064 | 0 | -0.108 | 0.52 |
| | O, O | 4.945 | 5.007 | 4.928 | 5.181 | -0.236 | 5.499 | -0.174 | 0 | -0.253 | 0.56 |
| | H, O | 0.542 | 0.730 | 0.681 | 0.849 | -0.307 | 16.554 | -0.119 | 0 | -0.168 | 0.519 |
| | OH, H | -0.471 | -0.467 | -0.471 | -0.451 | -0.02 | 11.111 | -0.016 | 0 | -0.02 | 0.26 |

* The high error arises from *H configuration not changing from the initial position during the first MLIP relaxation