

Benchmarking Machine-Learned Potentials for Adsorption on Pt and IrO₂ Surfaces Using OC20 and OMat24

Asmita Jana

Lawrence Berkeley National Laboratory

Fabrice Roncoroni

Lawrence Berkeley National Laboratory

Julie Fornaciari

Lawrence Berkeley National Laboratory

Aditi Krishnapriyan

University of California, Berkeley

David Prendergast

Lawrence Berkeley National Laboratory

Adam Weber

Lawrence Berkeley National Laboratory

Ethan Crumlin

Lawrence Berkeley National Laboratory

Jin Qian

`jqian2@lbl.gov`

Lawrence Berkeley National Laboratory

Research Article

Keywords: Machine Learning Interatomic Potentials, Adsorption Energy, Platinum, Iridium Dioxide, Water Splitting, Open Catalyst

Posted Date: April 17th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-9284189/v1>

License: © ⓘ This work is licensed under a Creative Commons Attribution 4.0 International License. [Read Full License](#)

Additional Declarations: No competing interests reported.

Benchmarking Machine-Learned Potentials for Adsorption on Pt and IrO₂ Surfaces Using OC20 and OMat24

Asmita Jana¹, Fabrice Roncoroni², Julie Fornaciari³,
Aditi S. Krishnapriyan⁴, David Prendergast², Adam Z. Weber³,
Ethan J. Crumlin^{1,5}, Jin Qian^{1*}

¹Chemical Sciences Division, Lawrence Berkeley National Laboratory,
Berkeley, CA, USA.

²Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley,
CA, USA.

³Energy Technologies, Lawrence Berkeley National Laboratory,
Berkeley, CA, USA.

⁴Chemical and Biomolecular Engineering, University of California
Berkeley, Berkeley, CA, USA.

⁵Advanced Light Source, Lawrence Berkeley National Laboratory,
Berkeley, CA, USA.

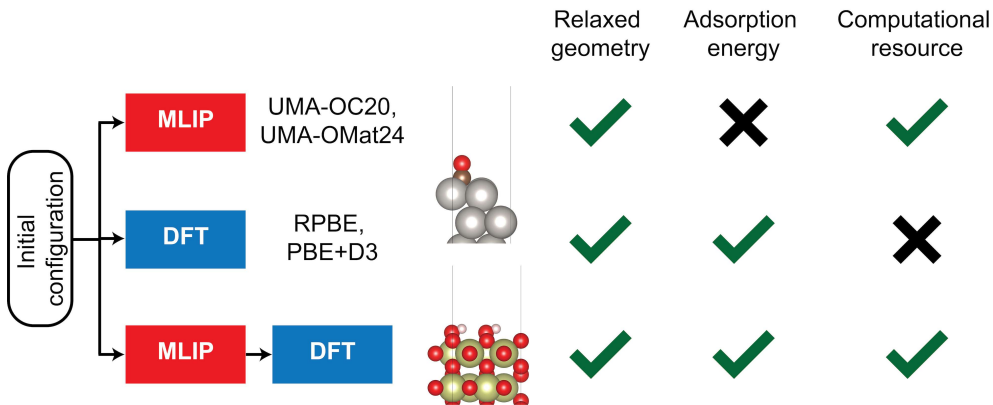
*Corresponding author(s). E-mail(s): jqian2@lbl.gov;

Abstract

Machine Learning Interatomic Potentials (MLIPs) enable first-principles accuracy in modeling complex catalytic interfaces at reduced cost. The Open Catalyst 2020 (OC20) and Open Materials 2024 (OMat24) datasets consist of density functional theory (DFT) data for adsorbates on metals and inorganic bulk materials, respectively. In this work, we benchmarked the Universal Model for Atoms (UMA) trained on the OC20 and OMat24 datasets with DFT calculations for adsorption energies on Pt and IrO₂, respectively. We evaluated adsorption energies of common adsorbates such as *H, *O, *CO, and *NO on Pt, and reaction intermediates in the water splitting reaction, such as *O, *OH, and *H, on IrO₂. UMA-OC20, trained using non-spin polarized DFT-RPBE energies with no van der Waals (vdW) corrections on metallic surfaces, reproduced the adsorption energies from the same flavor of DFT within 0.1 eV. However, the energy difference between UMA-OC20 and spin-polarized DFT was ~ 1.2 eV, with the

difference mainly arising from the reference gases. UMA-OMat24, trained using spin-polarized DFT-PBE with vdW corrections, predicted adsorption energies within 0.3 eV of the energies from the same flavor of DFT on IrO₂. When both the DFT flavor and geometry were kept fixed between the MLIPs and DFT, UMA-OC20 and UMA-OMat24 predicted adsorption energies within 0.1 and 0.2 eV of their corresponding DFT adsorption energies, respectively. The norm of coordinate differences between UMA-OC20 and DFT was ~ 0.1 Å for a system size of ~ 20 atoms, while it was < 0.6 Å for a system size of ~ 60 atoms, between UMA-OMat24 and DFT. MLIP requires considerably fewer (~ 6000 times less) CPU-hours compared to DFT. Thus, we recommend opting for an MLIP-followed-by-DFT procedure, as it not only reduces the total compute time but also ensures accurate geometry and energies.

Keywords: Machine Learning Interatomic Potentials, Adsorption Energy, Platinum, Iridium Dioxide, Water Splitting, Open Catalyst



1 Introduction

Machine Learning Interatomic Potentials (MLIPs) have substantially altered the domain of computational catalysis by facilitating quantum-mechanical accuracy at a fraction of the computational cost, opening up investigations in more complex interfaces with larger time and length scales.[1–6] MLIPs can predict adsorption energies, produce relaxed structures, and simulate surface dynamics accurately as a consequence of potential energy surfaces learned from density functional theory (DFT) data. Moreover, unlike traditional force fields, MLIPs can be systematically improved by fine-tuning or changing the last few layers in the model, feeding more training data, and/or using a better architecture.[7, 8] Thus, MLIPs have the potential to unlock applications ranging from long-timescale and large-length scale molecular

dynamics (MD) to high-throughput exploration of adsorption configurations.[1, 2, 9] Furthermore, evaluating and understanding atomistic phenomena at real, complex interfaces can help design the next-generation catalysts.

Progress in Machine Learning (ML)-accelerated computational chemistry is primarily due to the availability of large, diverse, open datasets with standardized tasks and splits. Datasets such as the Open Catalyst 2020 (OC20), Open Catalyst 2022 (OC22), and Open Catalyst 2025 (OC25) contain millions of DFT relaxations of interfacial systems corresponding to metals, metal oxides, and solid-liquid interfaces, respectively.[10–12] Similarly, the Open Materials 2024 (OMat24) contains over 100 million DFT structures and energies obtained from simulating inorganic bulk materials, including their non-equilibrium atomic configurations.[13] The Universal Model for Atoms (UMA) represents a family of pretrained MLIPs in the FAIRChem framework and is designed to capture transferable chemistries across heterogeneous catalysts.[14] Thus, UMA yields robust atomistic predictors that transfer across molecules, materials, surfaces, and interfaces. In general, data science research aimed at developing machine learning models with higher accuracy and requiring fewer computational resources accelerates computational chemistry research focused on materials discovery and property prediction.[14–17]

Despite the promise, MLIPs introduce new challenges in computational catalysis that need to be overcome before successful deployment. Modeling heterogeneous catalysts often involves computing adsorption energies of reaction intermediates, evaluating the transition states and corresponding activation energies, and then combining all structures and energies to obtain the reaction energy landscape and overall reaction rate.[18] To ensure accuracy in the final kinetic modeling, it is imperative that all energies are evaluated accurately (within ~ 0.1 eV is typical). Thus, in practice, using MLIPs for catalysis modeling applications is not trivial. MLIPs are sensitive to dataset biases and lack robustness outside the training data, necessitating careful selection of an MLIP for a given application. More importantly, MLIPs’ accuracy changes with the property evaluated and materials systems, and thus, they require uncertainty quantification and benchmarking before being deployed.[5, 14, 19] Systematic benchmarking of such models against DFT and experiment at the level of scientifically relevant reactions remains limited.[19–23] Platinum and iridium dioxide serve as benchmark systems for the hydrogen and oxygen evolution reactions (HER and OER) that underpin water electrolysis. Pt surfaces offer well-defined adsorption sites for $\ast\text{H}$ and $\ast\text{OH}$ intermediates, whereas rutile $\text{IrO}_2(110)$ provides the canonical pathway for OER species.[24–29] Reliable MLIPs for these materials could greatly accelerate mechanistic screening and reaction-network discovery.

In this work, we validate the OC20-trained and OMat24-trained UMA model for adsorption energetics on Pt on IrO_2 surfaces, respectively. Using DFT and available experimental data as references, we evaluate accuracy in adsorption energies, geometric fidelity, and site preference preservation. For Pt, we benchmarked common adsorbates such as $\ast\text{CO}$, $\ast\text{NO}$, $\ast\text{O}$, and $\ast\text{H}$. For $\text{IrO}_2(110)$, we analyze some water

splitting intermediates such as $\ast\text{H}$, $\ast\text{O}$, and $\ast\text{OH}$. The results demonstrate that for Pt adsorbates, UMA-OC20 achieves near-DFT accuracy (~ 0.1 eV difference) when compared to the same flavor of DFT (non-spin polarized) as the OC20 dataset. Comparing UMA-OC20 to a different flavor of DFT (spin-polarized) can yield large differences in adsorption energies (~ 1.2 eV). Similarly, the difference between adsorption energies from UMA-OMat24 and from DFT for adsorbates in IrO_2 is ~ 0.3 eV. Moreover, the norm of coordinate differences between the relaxed geometries from UMA-OC20 and from DFT was ~ 0.1 Å for a system size of ~ 20 atoms, while it was < 0.6 Å for a system size of ~ 60 atoms, between relaxed geometries from UMA-OMat24 and DFT. Leveraging MLIPs’ ability to perform geometry relaxation around ~ 6000 times faster than DFT and DFT’s ability to ensure accurate energies and geometries results in a recommendation of an MLIP-followed-by-DFT procedure for computational catalysis calculations.

2 Computational Methods

All calculations were performed using pretrained machine-learned interatomic potentials implemented in the FAIRChem framework. Two MLIPs were evaluated: UMA trained on OC20 dataset and UMA trained on OMat24 dataset.[10, 13, 14] UMA employs message-passing neural networks with equivariant feature representations to predict total energies and atomic forces directly from atomic structures.[14] We used UMA-OC20 for Pt adsorbates and UMA-OMat24 for IrO_2 adsorbates. The models were accessed through the FAIRChem Python API and coupled to the Atomic Simulation Environment (ASE) as calculators. The uma-s-1p1 checkpoint was implemented. LBFGS, or the limited memory version of the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm, was used to relax the structures with maximum force < 0.001 eV/Å for convergence. Single-point and geometry-optimization runs were conducted on representative Pt(111), Pt(110), and Pt(231) facets and on O-terminated rutile IrO_2 (110) slabs constructed with 15 Å of vacuum. The bottom 40% of the layers were fixed while the top 60% were allowed to relax.

To benchmark the adsorption energies generated using the datasets, we compared them to the adsorption energies we calculated using DFT calculations. We employed DFT calculations using the Vienna Ab initio Simulation Package (VASP) to obtain the optimized configurations.[30–32] We used the projector augmented wave (PAW) method and described the exchange-correlation effects using the generalized gradient approximation (GGA) as developed by Perdew, Burke, and Ernzerhof (PBE) plus van der Waals correction (PBE + D3) for IrO_2 adsorbates and the revised PBE (RPBE) from Hammer et al. for Pt adsorbates.[33–36] Spin-polarized calculations were performed for both the IrO_2 and Pt systems, but we also computed the non-spin-polarized energies for the Pt systems. An energy cutoff of 550 eV was used for all systems. For k-point meshes, we utilized $16 \times 16 \times 16$, $7 \times 7 \times 8$, and $1 \times 1 \times 1$ meshes for calculations of bulk Pt, bulk IrO_2 , and the reference gases (H_2 , O_2 , H_2O , NO , and CO) in a vacuum, respectively. To evaluate energies of the reference gases, we opted to place each gas molecule in a 15 Å cubic box. To represent adsorbate coverages

around 1/4, we chose 2×2 supercells for Pt(111) and Pt(110), and 1×2 supercells for O-terminated IrO₂(110). We chose a 3×3 supercell of Pt(111) to represent a 1/9 coverage. We opted for a 1×1 supercell for the irregularly shaped Pt(231). For Pt(111)-2×2, Pt(111)-3×3, Pt(110)-2×2, Pt(231)-1×1, and IrO₂(110)-1×2 surfaces, we used 11×11×1, 8×8×1, 6×10×1, 8×7×1, and 5×5×1 meshes, respectively after convergence tests. The bottom 40% of the layers were fixed while the top 60% were allowed to move during the geometry relaxation. We used 5 atomic layers for Pt(111), Pt(110), and IrO₂(110), and 10 layers for Pt(231). An additional 15 Å of vacuum was appended in the z direction to prevent undesirable neighboring interactions. We added dipole corrections in the direction perpendicular to the surface for slab calculations. We relaxed the structure containing surfaces to 10⁻⁶ eV of the total electronic energy.

3 Results and Discussion

To benchmark the MLIPs, we evaluated the adsorption energies for adsorbates on Pt and IrO₂ as representatives of the metals and metal oxides classes of materials. We wanted to ensure that the lattice constants are the same for calculations with MLIP and DFT. So, we used DFT to relax a bulk Pt and IrO₂ structure and then used the lattice parameter of the resulting relaxed bulk structure to design slabs for adsorption calculations, as shown in **Figure S1**. All adsorption energies, E_{ads} , were calculated by using [Equation 1](#).

$$E_{\text{ads}} = E(\text{adsorbate} + \text{slab}) - E(\text{slab}) - E(\text{gas reference}) \quad (1)$$

3.1 Adsorption on Pt

Since OC20 was trained explicitly for catalytic reactions on metal surface, it was chosen for simulating adsorption on Pt. We calculated the adsorption energies of CO, NO, O, and H adsorbates on Pt(111) and Pt(110) using UMA-OC20 and spin-polarized DFT, labelled Energy 1 and Energy 2 in [Figure 1a](#). In addition, we also included the experimental adsorption energies provided by Silbaugh and Campbell for reference.[37] The adsorption energies for Pt(111) and Pt(110) obtained using UMA-OC20, DFT, and experiments[37] are depicted in [Figure 2](#) and tabulated in **Table S1**. The Pt(111) and Pt(110) adsorption configurations obtained after DFT relaxation are depicted in [Figure 3](#) and [Figure 4](#), respectively. In order to compare directly with coverage-specific experiments,[37] note that the adsorbate coverage for O in Pt(111) is 1/9, while the coverage for all the other six cases is 1/4.

Before we delve into a comparison across all the methods of adsorption energy calculation, we want to point out the differences between all the methods. First, our DFT calculations in [Figure 2](#) and **Table S1** contain spin polarization, with no van der Waals correction. This is in contrast to MLIPs. The OC20 dataset is calculated with RPBE without spin polarization and van der Waals D3 corrections.[10] The second point of difference arises from the difference in geometries. We ensured that the

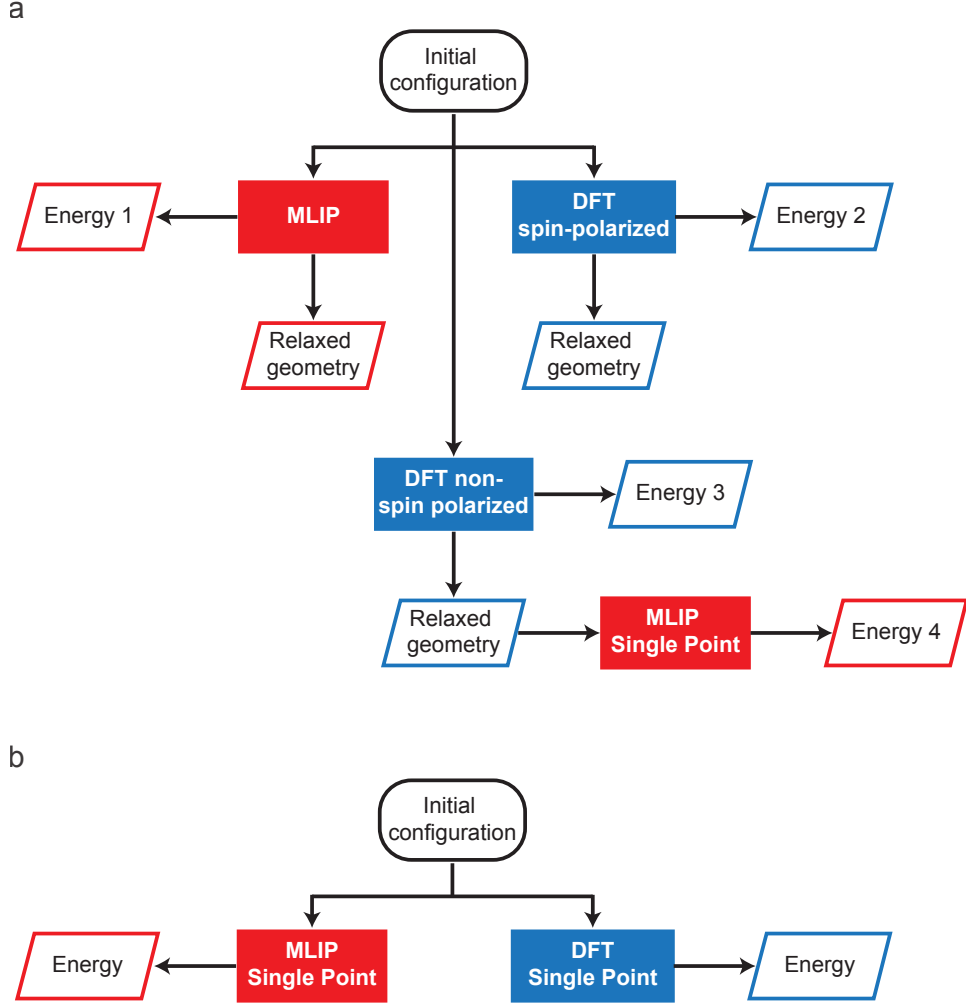


Fig. 1 a. The workflow used for Pt(111) and Pt(110). Both spin-polarized (**Figure 2**) and non-spin polarized (**Figure 5**) DFT were used to compare with the MLIP relaxation. Additionally, MLIP single point calculations on the same geometry as the non-spin polarized DFT calculation (**Figure 6**) provide the lowest error. b. The workflow used for Pt(231). Only single point calculations were done on a static geometry (**Figure 8**)

lattice parameter for Pt is constant across all of the calculation methods by overwriting the lattice parameter in the ASE calculator for MLIPs with the lattice parameter that we obtained using DFT calculations (**Figure S1**). However, since each MLIP and DFT calculations relax the geometries independently, they can result in slightly different relaxed geometries. To evaluate the difference in atomic positions in the relaxed configurations obtained from MLIPs and DFT, we computed the Euclidean

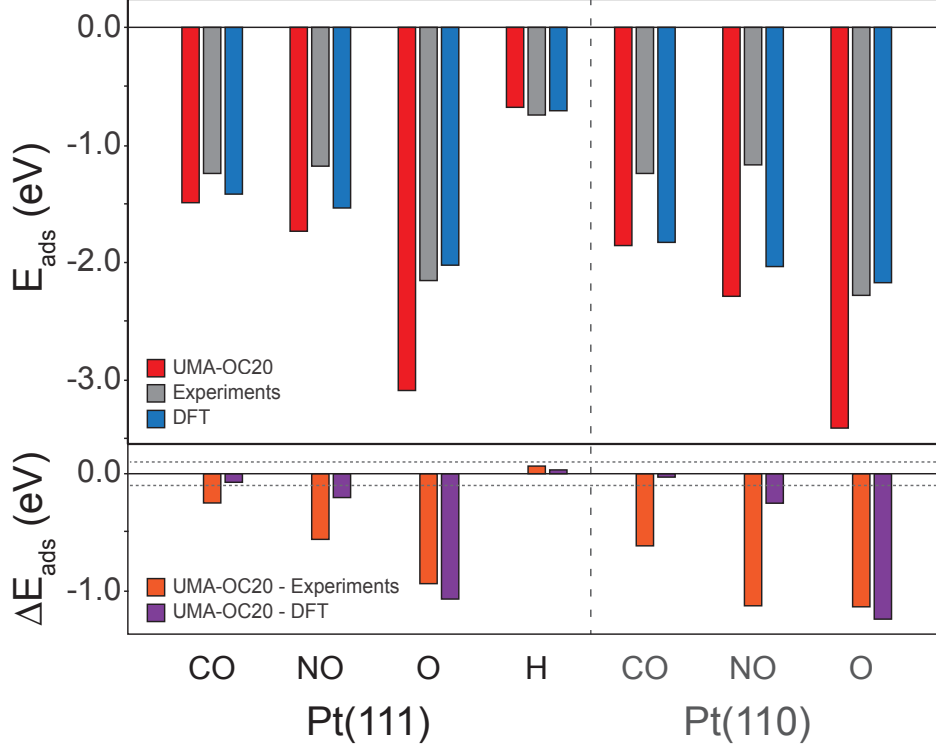


Fig. 2 Ground state from each method: Adsorption energies of adsorbates on Pt(111) and Pt(110) calculated using UMA-OC20 (Energy 1 in [Figure 1a](#)) are benchmarked with spin-polarized DFT calculations (Energy 2 in [Figure 1a](#)) and experimental results from Silbaugh and Campbell.[\[37\]](#) Horizontal dashed lines represent the bounds of acceptable error for adsorption energy, ± 0.1 eV. The vertical dashed line separates the Pt surface facets—Pt(111) and Pt(110)

norm of the coordinate differences (flattened over all atoms and coordinates) as given by [Equation 2](#).

$$d_{AB} = \sqrt{\sum_{i=1}^N \left[(x_i^A - x_i^B)^2 + (y_i^A - y_i^B)^2 + (z_i^A - z_i^B)^2 \right]} \quad (2)$$

Where d_{AB} is the Euclidean norm of two configurations A and B . (x_i^A, y_i^A, z_i^A) and (x_i^B, y_i^B, z_i^B) are the cartesian coordinates of the i th atom in configurations A and B , respectively and N represents the total number of atoms in each of the configuration. The Euclidean norm between the relaxed configurations obtained from UMA-OC20 and spin-polarized DFT is 0.07–0.18 Å, and is tabulated in [Table S1](#).

Across all the adsorbates shown in [Figure 2](#), we observed the highest differences

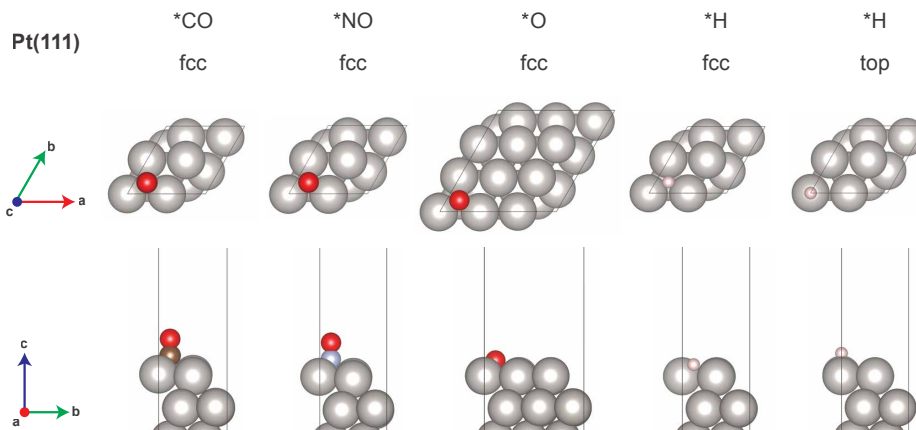


Fig. 3 The Pt(111) adsorption configurations obtained after DFT relaxation. The structures obtained after MLIP relaxation are indistinguishable from the DFT relaxed structures and hence, are not displayed. We quantified the subtle difference in structures between MLIP and DFT in **Tables S1** and **S2**

in adsorption energies $\sim 1\text{--}1.2$ eV between the UMA-OC20 and our DFT calculations for $\ast\text{O}$ in Pt(111) and Pt(110). We attribute the difference to OC20 not using spin-polarized calculations, which is crucial for simulating O-containing entities, including getting the ground state for O_2 . However, we opted for spin-polarized DFT calculations. Thus, the difference in spin polarization between UMA-OC20 and our DFT calculations results in the difference in adsorption energies of all adsorbates in general, and $\ast\text{O}$ adsorption energies, in particular. Other than $\ast\text{O}$, the highest difference in adsorption energies is around 0.2 eV. Furthermore, another source of difference in energies can be attributed to the different geometries resulting from geometry relaxations in MLIPs and DFT, although the lattice parameter is kept fixed in both. This effect is relatively minor, as evidenced by the Euclidean norm of the coordinate differences being ~ 0.1 Å for a system size of ~ 20 atoms from **Table S1**. Additionally, the energies of reference gases are calculated as a linear combination of N_2 , H_2O , CO , and H_2 in the OC20 dataset.[10] The difference between the energies of the reference gases obtained from DFT and the energies obtained from the linear combination employed by OC20 also contributes to the error observed (**Table S5**).

While results from **Figure 2** help us understand how different our independent ground state DFT energies are from MLIPs, we wanted to evaluate how closely UMA-OC20 energies match our DFT energies if our hypothesized sources of differences were eliminated. To achieve that, we calculated the non-spin polarized adsorption energies using DFT, labelled Energy 3 in **Figure 1a**, eliminating any difference in DFT flavor. The resulting adsorption energies and their differences are depicted in **Figure 5** and tabulated in **Table S2**. We now observed much closer agreement; in fact, the highest difference in adsorption energies was only ~ 0.1 eV, well within the accepted

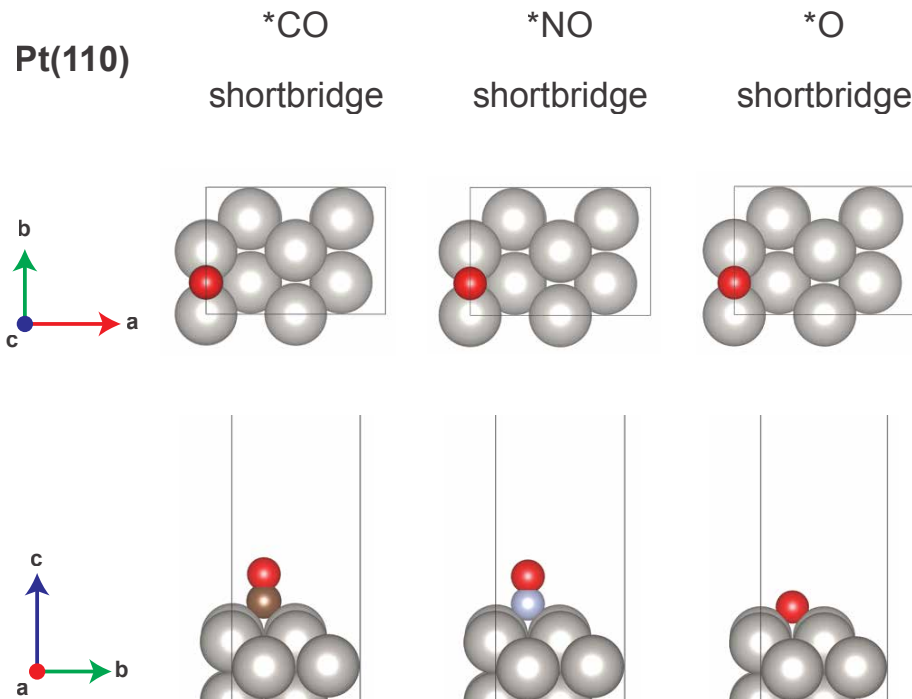


Fig. 4 The Pt(110) adsorption configurations obtained after DFT relaxation. The structures obtained after MLIP relaxation are indistinguishable from the DFT relaxed structures and hence, are not displayed. We quantified the subtle difference in structures between MLIP and DFT in **Tables S1** and **S2**

error for adsorption energies calculated using DFT. Thus, eliminating the difference in DFT flavor eliminated most of the difference in adsorption energies we observed in **Figure 2**. This observation also aligns with our assertion that geometry differences are a relatively minor source of difference in **Figure 2**. Additionally, we tabulated the energies of adsorbate + slab, slab, and reference gas, for the spin-polarized DFT, non-spin polarized DFT, and UMA-OC20 in **Table S5**. While the energies of the adsorbate + slab, slab, and reference gas of UMA-OC20 do not match those from non-spin polarized DFT, the error cancellation ensures that the adsorption energy of UMA-OC20 matches that of non-spin polarized DFT. We also observed that the difference in adsorption energies between spin-polarized and non-spin polarized DFT calculations (~ 0.3 – 0.6 eV) arises mainly (90–100%) from the gas phase reference calculation (**Table S6**). On the contrary, the Euclidean norm of the coordinate differences between spin-polarized and non-spin polarized DFT calculations of the slab with adsorbate is negligible (≤ 0.04 Å for a system size of ~ 20 atoms). This implies that the impact of adding spin polarization on the relaxed geometry is minimal.

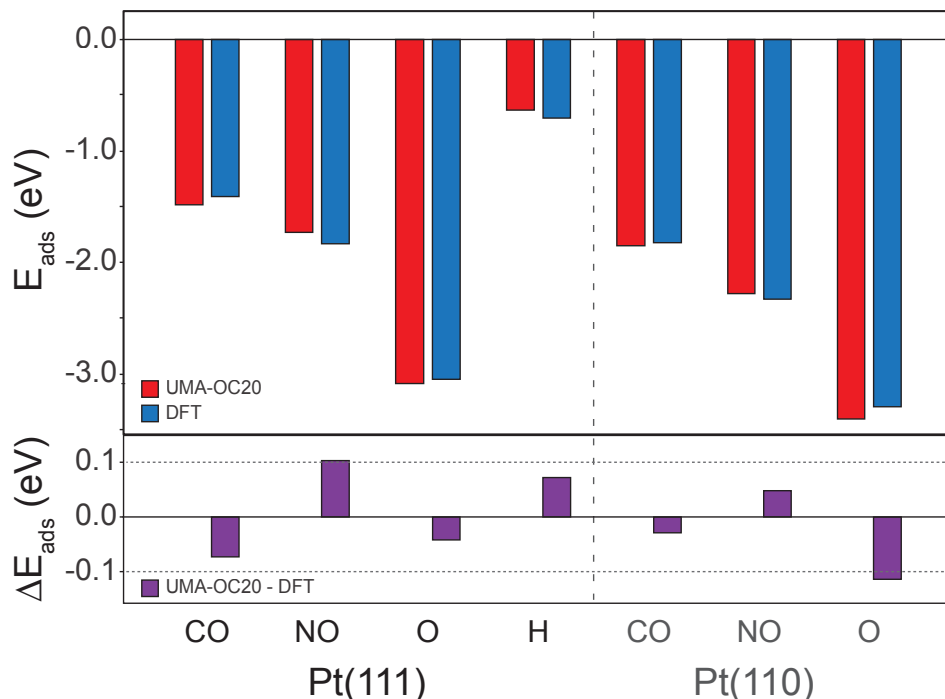


Fig. 5 With the same DFT flavor and different geometries: Adsorption energies of adsorbates on Pt(111) and Pt(110) calculated using UMA-OC20 (Energy 1 in [Figure 1a](#)) are benchmarked with non-spin polarized DFT calculations (Energy 3 in [Figure 1a](#)). Horizontal dashed lines represent the bounds of acceptable error for adsorption energy, ± 0.1 eV. The vertical dashed line separates the Pt surface facets—Pt(111) and Pt(110)

Next, instead of using UMA-OC20 for geometry optimization, we used it to calculate single point energies for structures obtained from our non-spin polarized DFT calculations, labelled Energy 4 in [Figure 1a](#), thereby removing any differences in geometry. The resulting adsorption energies and their differences are depicted in [Figure 6](#) and tabulated in [Table S3](#). We observed good agreement, as expected, and the highest difference in adsorption energies was ~ 0.1 eV, similar to the difference obtained in [Figure 5](#). We want to emphasize that since the effect of the geometry difference is minor, fixing the geometry did not change the difference in adsorption energy significantly.

These sets of benchmarks indicate that UMA-OC20 yields accurate energies when systems do not require spin-polarized calculations to capture the ground state energy. Moreover, in such cases, its prediction of adsorption sites and relaxed geometry is accurate enough to serve as an inexpensive preliminary calculation. We found that a traditional DFT calculation requires ~ 6000 times CPU-hours in these systems compared to an MLIP calculation. Thus, using MLIPs for a preliminary calculation followed by a shorter DFT calculation is more efficient while providing the desired

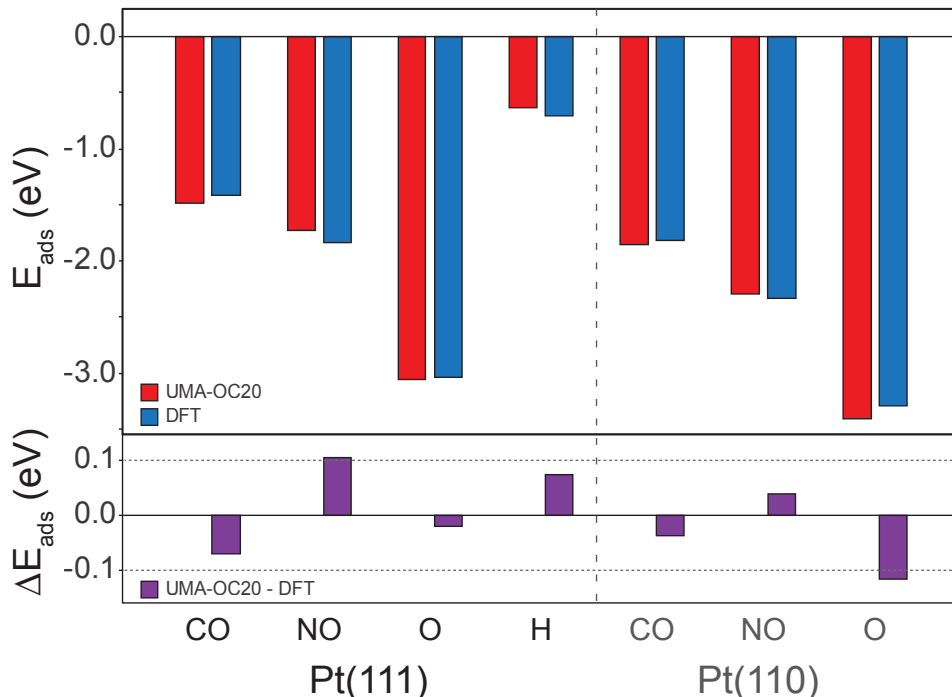


Fig. 6 With the same DFT flavor and the same geometries: Adsorption energies of adsorbates on Pt(111) and Pt(110) calculated using UMA-OC20 (Energy 4 in [Figure 1a](#)) are benchmarked with non-spin polarized DFT calculations (Energy 3 in [Figure 1a](#)). Horizontal dashed lines represent the bounds of acceptable error for adsorption energy, ± 0.1 eV. The vertical dashed line separates the Pt surface facets—Pt(111) and Pt(110)

accuracy, compared to one long DFT calculation.

To investigate how accurately MLIPs can capture the adsorption energies of the adsorbates on an unconventional surface facet, we evaluated the energies for Pt(231) using UMA-OC20 and non-spin polarized DFT. We placed the adsorbate molecule 2 Å away from the surface on three top sites corresponding to the first, second, and third layer (site 1, 2, and 3, respectively), which are exposed to the vacuum. The configurations of *O on these three sites are depicted in [Figure 7](#); other adsorbates also used the same sites. We opted for a single point calculation for both MLIP and non-spin polarized DFT, instead of geometry relaxation ([Figure 1b](#)). Thus, both sets of calculations are performed on the same fixed geometry and with the same DFT flavor. Because we chose not to relax the geometries, the energies for Pt(231) cannot technically be classified as adsorption energies but rather interaction energies with the adsorbate molecule artificially fixed 2 Å away from the surface. The results from these calculations are depicted in [Figure 8](#) and [Table S4](#).

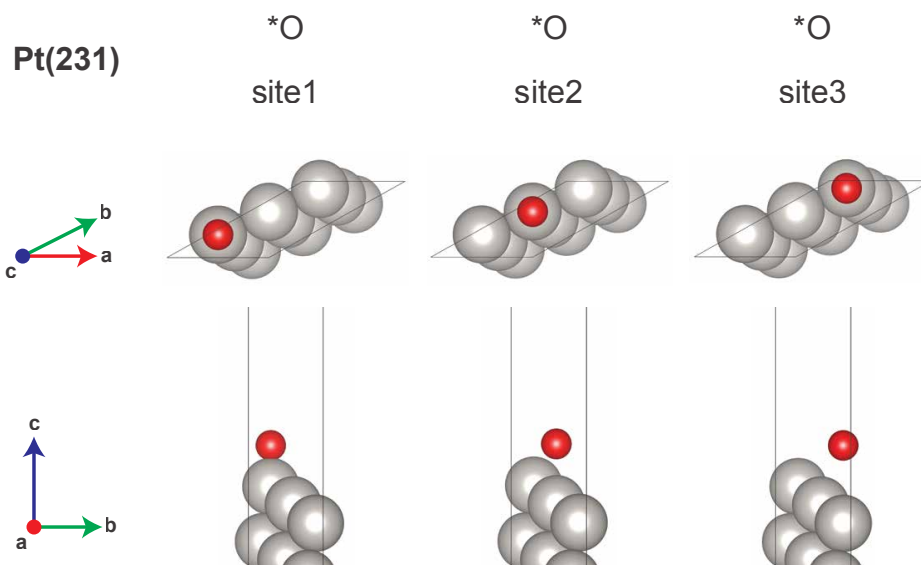


Fig. 7 The Pt(231) configurations corresponding to the adsorbate molecule being placed on the three top sites are depicted for $^*\text{O}$, as an example. The same sites are used for the other adsorbates as well

Since the interactions between the adsorbate and the Pt(231) surface are calculated for static structures without geometry optimizations, some of the energies are positive. The maximum energy difference we observe is around ~ 0.1 eV, well within the DFT error for adsorption. Thus, we concluded that UMA-OC20 is well-equipped to capture the energetics of even an unconventional system like Pt(231).

3.2 Adsorption on IrO_2

To benchmark the MLIPs for metal oxides, we chose to study water splitting adsorbates on $\text{IrO}_2(110)$. While the OC22 dataset is technically intended for metal oxide-based catalysts, we opted for the OMat24 due to the lack of publicly available UMA models trained on OC22.[11, 13] In spite of OMat24 being trained on bulk inorganic materials and not on oxide surfaces, we show that it can still accurately capture the surface energetics in IrO_2 . We hypothesize that the large training set consisting of near-equilibrium and out-of-equilibrium structures obtained via perturbations results in the model being capable of predicting even surface geometries and energetics.

Just like the Pt systems, to benchmark the UMA-OMat24 results, we performed DFT calculations at the same level of theory as OMat24. We used spin-polarized DFT with PBE, with dipole corrections and van der Waals corrections. We investigated a 1×2 supercell of O-terminated $\text{IrO}_2(110)$, which exposes two O-top sites for adsorption. We calculated the adsorption energies of H, O, and OH adsorbates in six

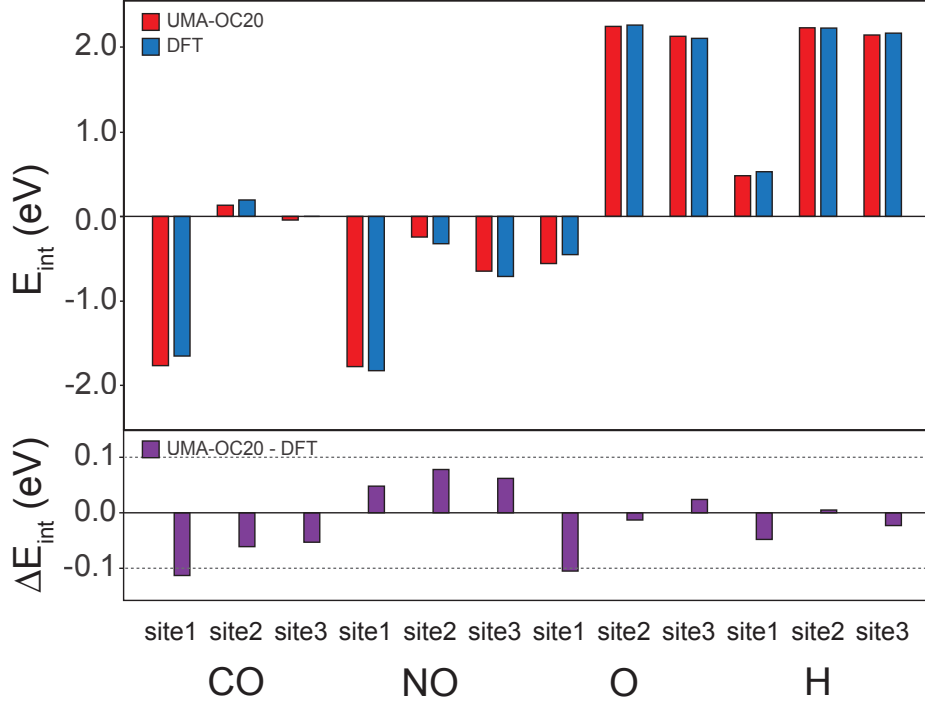


Fig. 8 With the same DFT flavor and the same geometries: Adsorption energies of adsorbates on Pt(231) calculated using UMA-OC20 are benchmarked with DFT calculations (both Energy terms in [Figure 1b](#)). Horizontal dashed lines represent the bounds of acceptable error for adsorption energy, ± 0.1 eV

combinations on the two sites: H, -; H, H; O, -; O, O, H, O; and OH, H; tabulated in **Table S7**. We computed the MLIP and DFT energies using the procedure depicted in [Figure 9](#). The $\text{IrO}_2(110)$ adsorption configurations obtained after DFT and MLIP relaxations are depicted in [Figure 10](#).

First, we used DFT to optimize the IrO_2 bulk structure to yield the lattice parameter. Keeping that lattice parameter fixed, we constructed the 1×2 supercell of O-terminated $\text{IrO}_2(110)$ slab, as described in **Figure S1**. After placing the six adsorbate combinations on the two O-top sites, we used UMA-OMat24 MLIP to relax the geometries and obtain energies, labelled Energy R1 in [Figure 9](#) and [Figure 11](#). Next, the structure from MLIP (R1) was taken as an initial structure and subjected to a geometry optimization using DFT. The energies from this DFT calculation are labelled Energy DFT in [Figure 9](#) and [Figure 11](#). Furthermore, a single point calculation of the final structure obtained from DFT is performed using MLIP to obtain Energy SP as shown in [Figure 9](#) and [Figure 11](#). This final structure is finally subjected to another geometry relaxation with the MLIP, and we obtained Energy R2 as depicted in [Figure 9](#) and [Figure 11](#).

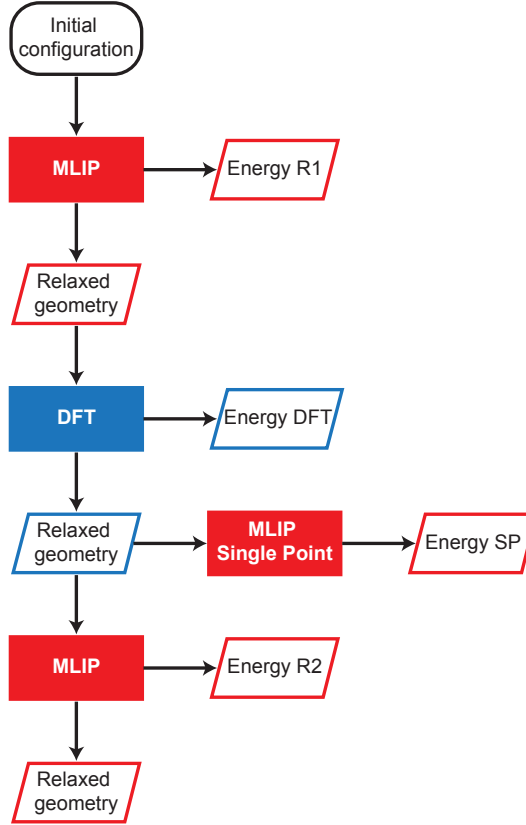


Fig. 9 The workflow used for IrO₂(110). The first MLIP relaxation (R1), DFT relaxation (DFT), MLIP single point calculations on the resulting DFT relaxed geometry (SP), and second MLIP relaxation (R2) are all compared

While MLIP (R1) and MLIP (R2) calculations result in different geometries compared to DFT, MLIP (SP) and DFT energies share the same geometry. This explains why the difference between MLIP (SP) and DFT adsorption energies is the lowest at <0.2 eV. Next, the difference between MLIP (R1) and DFT indicates how closely the MLIP can, in a first try, get to the minimum energy configuration. From [Figure 11](#), we observed that other than the H₁- configuration, MLIP (R1) captures the adsorption energetics to within ~ 0.3 eV of the DFT values. For the H₁- configuration, the adsorption energy difference between MLIP (R1) and DFT is ~ 0.9 eV. This large difference in adsorption energies cannot be explained by the norm of coordinate differences (9.13 Å) alone. We attribute this large difference to the angular difference also; while the H-O-Ir angle in the DFT relaxed structure is 108° , MLIP (R1) yields 180° .

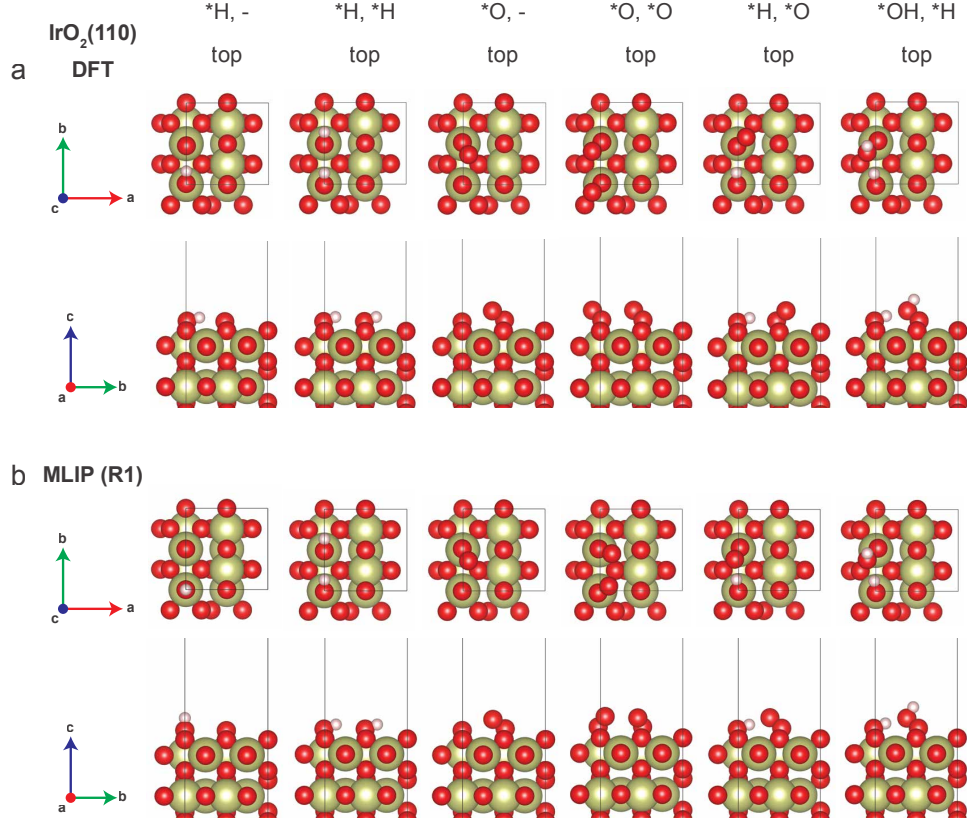


Fig. 10 The IrO₂(110) adsorption configurations obtained after a. DFT relaxation and b. MLIP (R1) relaxation. The structures obtained after MLIP (R2) relaxation are indistinguishable from the DFT relaxed structures and hence, are not displayed. We quantified the subtle difference in structures between MLIP and DFT in **Table S7**

Overall, the Euclidean norm of coordinate differences between MLIP (R1) and DFT is $< 17 \text{ \AA}$ for a system size of ~ 60 atoms (**Table S7**). MLIP can serve as a preliminary calculation to quickly converge to an intermediate relaxed geometry, as shown in **Figure 10b**, before we funnel it to a highly accurate DFT calculation. In fact, this strategy underlines why we chose to perform DFT calculations after the MLIP (R1) calculation. Finally, after the DFT calculation, we subjected the final geometry to a further MLIP relaxation (R2) to investigate if the MLIP accepted the geometry as the minimum energy configuration or tried to predict an alternative one. We observed that the MLIP (R2) does not make any substantial changes from the DFT relaxed structure (Norm $< 0.6 \text{ \AA}$ for a system size of ~ 60 atoms). Unsurprisingly, we note that the H, - configuration, which the MLIP failed to relax in the first try (Norm is $9.13 \text{ \AA}$ in R1), is now well captured by the MLIP in the second attempt (Norm is $0.24 \text{ \AA}$ in R2). Moreover, the difference in adsorption energies between MLIP (R2)

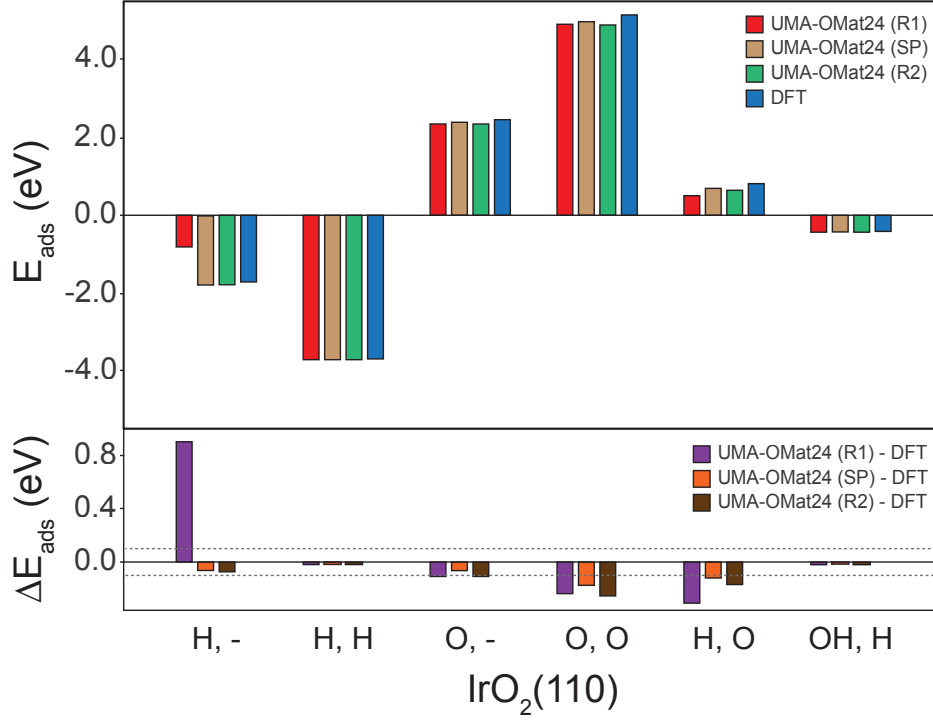


Fig. 11 MLIP + DFT for $\text{IrO}_2(110)$: Adsorption energies of adsorbates on $\text{IrO}_2(110)$ calculated using UMA-OMat24 are benchmarked with DFT calculations. Horizontal dashed lines represent the bounds of acceptable error for adsorption energy, ± 0.1 eV

and DFT is ~ 0.3 eV, similar to MLIP (R1). In other words, even when the MLIP relaxes the geometry to a configuration similar to the DFT relaxed configuration, as is the case in MLIP (R2) with $\text{Norm} < 0.6$ Å, the MLIP adsorption energies can still differ from DFT ones substantially. This further underscores the necessity to perform quick DFT calculations after MLIP to obtain accurate energies and geometries.

4 Conclusion

In this work, we used UMA with OC20 and OMat24 to benchmark the adsorption energetics on Pt and IrO_2 surfaces, respectively. We used UMA-OC20 to investigate adsorption on Pt(111), Pt(110), and Pt(231) surfaces. UMA-OC20 predicted adsorption energies within ~ 0.1 eV of non-spin polarized DFT adsorption energies, well within the acceptable error. However, the difference between adsorption energies from UMA-OC20 and spin-polarized DFT, a different DFT flavor from OC20, was ~ 1.2 eV. We attributed the large difference in adsorption energy to the difference in spin-polarized and non-spin polarized energies of the O_2 and NO gas references.

Moreover, since gases like O_2 and NO require spin polarization for accurate energies, we argue that UMA-OC20 alone is insufficient to describe their energetics. Thus, UMA-OC20 yields accurate energies when systems do not require spin-polarized calculations to capture the ground state energy. From a geometry relaxation perspective, UMA-OC20 predicted structures very similar to both spin-polarized and non-spin polarized DFT calculations (Norm ~ 0.1 Å for a system size of ~ 20 atoms). Thus, the UMA-OC20 MLIP is well-suited to serve as an inexpensive preliminary calculation to yield an intermediate geometry that can be funneled into a shorter DFT calculation to get accurate surface energetics and geometries. Since geometry optimization steps in DFT are frequently the computational bottleneck, performing an MLIP-followed-by-DFT procedure cuts down the overall computational time substantially while still maintaining accurate energies.

We tested this MLIP-followed-by-DFT procedure on a different MLIP and a different system; we used UMA-OMat24 MLIP on $\text{IrO}_2(110)$ surface. UMA-OMat24 predicted adsorption energies within ~ 0.3 eV of DFT adsorption energies, which is higher than the acceptable error. Even when provided with DFT relaxed geometries as initial configuration, it yielded relaxed geometries which differed from the DFT relaxed geometries by a norm < 0.6 Å for a system size of ~ 60 atoms. However, when applied on the same (DFT relaxed) geometries, the difference between adsorption energies from UMA-OMat24 (single point) and DFT was reduced to ~ 0.2 eV, still higher than the community’s acceptable error (0.1 eV). This underscores the importance of performing a subsequent DFT calculation to obtain accurate energies even when the geometries predicted by the MLIP are the same as the geometries from DFT. Moreover, the subsequent DFT relaxation after UMA-OMat24 was much faster compared to a traditional DFT relaxation without a previous MLIP relaxation step.

In summary, we urge practitioners of MLIPs in the domain of computational chemistry to opt for an MLIP-followed-by-DFT procedure if they need accurate energies, geometries, forces, and electronic structures. More such studies using other MLIPs on other systems are needed to support our recommendation, and we look forward to more benchmarking papers on MLIPs. Furthermore, fine-tuning or active learning can be used to increase the accuracy of adsorption energies predicted by MLIPs.[7, 8] However, the steep computational cost to train and loss of generalization can prevent widespread application in favor of the easily available pretrained MLIPs. Finally, while we have tested MLIPs for adsorption on simple gas/solid interfaces, MLIPs can create a vast impact on evaluating more complex gas/liquid/solid interfaces, especially those in electrochemistry. To accomplish this, we need to design MLIPs that can evaluate long-range interactions, as such long-range electrostatic interactions are common in electrochemistry.[38–41] It is also imperative to design workflows for MD calculations using MLIPs that can evaluate the effect of applied potential.[42–45] As more accurate and computationally efficient ML models get developed, benchmarked, and adapted by the computational chemistry community, we get closer to creating the required tools and computational workflow to evaluate atomistic phenomena at real, complex interfaces – a goal with the potential to unleash the next-generation of

energy sciences.

5 Declarations

5.1 Funding

This work was funded in part by the Office of Science, Office of Basic Energy Sciences in the Chemical Sciences, Geosciences, and Biosciences subprogram at Lawrence Berkeley National Laboratory under contract #DE-AC02-05CH11231. This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC award BES-ERCAP0031518.

5.2 Conflict of interest/Competing interests

There are no conflicts to declare.

5.3 Ethics approval and consent to participate

Not applicable

5.4 Consent for publication

All authors consent for the publication.

5.5 Data availability

All data generated or analysed during this study are included in this published article [and its supplementary information files].

5.6 Materials availability

Not applicable

5.7 Code availability

Not applicable

5.8 Author contribution

Conceptualization, A. J. and J. Q.; methodology, A. J., A. S. K., D. P., and J. Q.; investigation, A. J. and J. Q.; writing – original draft, A. J.; writing – review and editing, all authors; funding acquisition, J. Q. and A. Z. W.; supervision, J. Q.

References

- [1] Omranpour, A., Elsner, J., Lausch, K.N., Behler, J.: Machine Learning Potentials for Heterogeneous Catalysis. *ACS Catalysis* **15**(3), 1616–1634 (2025) <https://doi.org/10.1021/acscatal.4c06717> . Accessed 2026-01-20
- [2] Mou, T., Pillai, H.S., Wang, S., Wan, M., Han, X., Schweitzer, N.M., Che, F., Xin, H.: Bridging the complexity gap in computational heterogeneous catalysis with machine learning. *Nature Catalysis* **6**(2), 122–136 (2023) <https://doi.org/10.1038/s41929-023-00911-w> . Accessed 2026-01-20
- [3] Guan, Y., Chaffart, D., Liu, G., Tan, Z., Zhang, D., Wang, Y., Li, J., Ricardez-Sandoval, L.: Machine learning in solid heterogeneous catalysis: Recent developments, challenges and perspectives. *Chemical Engineering Science* **248**, 117224 (2022) <https://doi.org/10.1016/j.ces.2021.117224> . Accessed 2026-01-20
- [4] Erdem Günay, M., Yıldırım, R.: Recent advances in knowledge discovery for heterogeneous catalysis using machine learning. *Catalysis Reviews* **63**(1), 120–164 (2021) <https://doi.org/10.1080/01614940.2020.1770402> . Accessed 2026-01-20
- [5] SchlexerLamoureux, P., Winther, K.T., GarridoTorres, J.A., Streibel, V., Zhao, M., Bajdich, M., Abild-Pedersen, F., Bligaard, T.: Machine Learning for Computational Heterogeneous Catalysis. *ChemCatChem* **11**(16), 3581–3601 (2019) <https://doi.org/10.1002/cctc.201900595> . Accessed 2026-01-20
- [6] Goldsmith, B.R., Esterhuizen, J., Liu, J., Bartel, C.J., Sutton, C.: Machine learning for heterogeneous catalyst design and discovery. *AIChE Journal* **64**(7), 2311–2323 (2018) <https://doi.org/10.1002/aic.16198> . Accessed 2026-01-20
- [7] Schaaf, L.L., Fako, E., De, S., Schäfer, A., Csányi, G.: Accurate energy barriers for catalytic reaction pathways: an automatic training protocol for machine learning force fields. *npj Computational Materials* **9**(1), 180 (2023) <https://doi.org/10.1038/s41524-023-01124-2> . Accessed 2026-01-20
- [8] Perego, S., Bonati, L.: Data efficient machine learning potentials for modeling catalytic reactivity via active learning and enhanced sampling. *npj Computational Materials* **10**(1), 291 (2024) <https://doi.org/10.1038/s41524-024-01481-6> . Accessed 2026-01-20
- [9] Westermayr, J., Gastegger, M., Menger, M.F.S.J., Mai, S., González, L., Marquetand, P.: Machine learning enables long time scale molecular photodynamics simulations. *Chemical Science* **10**(35), 8100–8107 (2019) <https://doi.org/10.1039/C9SC01742A> . Accessed 2026-01-20
- [10] Chanussot, L., Das, A., Goyal, S., Lavril, T., Shuaibi, M., Riviere, M., Tran, K., Heras-Domingo, J., Ho, C., Hu, W., Palizhati, A., Sriram, A., Wood, B., Yoon, J., Parikh, D., Zitnick, C.L., Ulissi, Z.: Open Catalyst 2020 (OC20) Dataset and

- Community Challenges. *ACS Catalysis* **11**(10), 6059–6072 (2021) <https://doi.org/10.1021/acscatal.0c04525> . Accessed 2026-01-20
- [11] Tran, R., Lan, J., Shuaibi, M., Wood, B.M., Goyal, S., Das, A., Heras-Domingo, J., Kolluru, A., Rizvi, A., Shoghi, N., Sriram, A., Therrien, F., Abed, J., Voznyy, O., Sargent, E.H., Ulissi, Z., Zitnick, C.L.: The Open Catalyst 2022 (OC22) Dataset and Challenges for Oxide Electrocatalysts. *ACS Catalysis* **13**(5), 3066–3084 (2023) <https://doi.org/10.1021/acscatal.2c05426> . Accessed 2026-01-20
- [12] Sahoo, S.J., Maraschin, M., Levine, D.S., Ulissi, Z., Zitnick, C.L., Varley, J.B., Gauthier, J.A., Govindarajan, N., Shuaibi, M.: The Open Catalyst 2025 (OC25) Dataset and Models for Solid-Liquid Interfaces. *arXiv*. Version Number: 1 (2025). <https://doi.org/10.48550/ARXIV.2509.17862> . <https://arxiv.org/abs/2509.17862> Accessed 2026-01-20
- [13] Barroso-Luque, L., Shuaibi, M., Fu, X., Wood, B.M., Dzamba, M., Gao, M., Rizvi, A., Zitnick, C.L., Ulissi, Z.W.: Open Materials 2024 (OMat24) Inorganic Materials Dataset and Models. *arXiv*. Version Number: 1 (2024). <https://doi.org/10.48550/ARXIV.2410.12771> . <https://arxiv.org/abs/2410.12771> Accessed 2026-01-20
- [14] Wood, B.M., Dzamba, M., Fu, X., Gao, M., Shuaibi, M., Barroso-Luque, L., Abdelmaqsoud, K., Gharakhanyan, V., Kitchin, J.R., Levine, D.S., Michel, K., Sriram, A., Cohen, T., Das, A., Rizvi, A., Sahoo, S.J., Ulissi, Z.W., Zitnick, C.L.: UMA: A Family of Universal Models for Atoms. *arXiv*. Version Number: 1 (2025). <https://doi.org/10.48550/ARXIV.2506.23971> . <https://arxiv.org/abs/2506.23971> Accessed 2026-01-20
- [15] Batatia, I., Kovács, D.P., Simm, G.N.C., Ortner, C., Csányi, G.: MACE: Higher Order Equivariant Message Passing Neural Networks for Fast and Accurate Force Fields. *arXiv*. Version Number: 2 (2022). <https://doi.org/10.48550/ARXIV.2206.07697> . <https://arxiv.org/abs/2206.07697> Accessed 2026-01-20
- [16] Liao, Y.-L., Wood, B., Das, A., Smidt, T.: EquiformerV2: Improved Equivariant Transformer for Scaling to Higher-Degree Representations. *arXiv*. Version Number: 3 (2023). <https://doi.org/10.48550/ARXIV.2306.12059> . <https://arxiv.org/abs/2306.12059> Accessed 2026-01-20
- [17] Fu, X., Wood, B.M., Barroso-Luque, L., Levine, D.S., Gao, M., Dzamba, M., Zitnick, C.L.: Learning Smooth and Expressive Interatomic Potentials for Physical Property Prediction. *arXiv*. Version Number: 2 (2025). <https://doi.org/10.48550/ARXIV.2502.12147> . <https://arxiv.org/abs/2502.12147> Accessed 2026-01-20
- [18] Motagamwala, A.H., Dumesic, J.A.: Microkinetic Modeling: A Tool for Rational Catalyst Design. *Chemical Reviews* **121**(2), 1049–1076 (2021) <https://doi.org/10.1021/acs.chemrev.0c00394> . Accessed 2026-01-20

- [19] Kempen, L.H.E., Cheula, R., Andersen, M.: How accurate are foundational machine learning interatomic potentials for heterogeneous catalysis? arXiv. Version Number: 1 (2025). <https://doi.org/10.48550/ARXIV.2512.16702> . <https://arxiv.org/abs/2512.16702> Accessed 2026-01-20
- [20] Abed, J., Kim, J., Shuaibi, M., Wander, B., Duijf, B., Mahesh, S., Lee, H., Gharakhanyan, V., Hoogland, S., Irtem, E., Lan, J., Schouten, N., Vijayakumar, A.U., Hattnick-Simpers, J., Kitchin, J.R., Ulissi, Z.W., Vugt, A., Sargent, E.H., Sinton, D., Zitnick, C.L.: Open Catalyst Experiments 2024 (OCx24): Bridging Experiments and Computational Models. arXiv. Version Number: 1 (2024). <https://doi.org/10.48550/ARXIV.2411.11783> . <https://arxiv.org/abs/2411.11783> Accessed 2026-01-20
- [21] Moon, J., Jeon, U., Choung, S., Han, J.W.: CatBench framework for benchmarking machine learning interatomic potentials in adsorption energy predictions for heterogeneous catalysis. *Cell Reports Physical Science* **6**(12), 102968 (2025) <https://doi.org/10.1016/j.xcrp.2025.102968> . Accessed 2026-01-20
- [22] Felton, K.C., Rittig, J.G., Lapkin, A.A.: Summit: Benchmarking Machine Learning Methods for Reaction Optimisation. *Chemistry–Methods* **1**(2), 116–122 (2021) <https://doi.org/10.1002/cmt.d.202000051> . Accessed 2026-01-20
- [23] Bozal-Ginesta, C., Pablo-García, S., Choi, C., Tarancón, A., Aspuru-Guzik, A.: Developing machine learning for heterogeneous catalysis with experimental and computational data. *Nature Reviews Chemistry* **9**(9), 601–616 (2025) <https://doi.org/10.1038/s41570-025-00740-4> . Accessed 2026-01-20
- [24] Li, C., Baek, J.-B.: Recent Advances in Noble Metal (Pt, Ru, and Ir)-Based Electrocatalysts for Efficient Hydrogen Evolution Reaction. *ACS Omega* **5**(1), 31–40 (2020) <https://doi.org/10.1021/acsomega.9b03550> . Accessed 2026-01-20
- [25] Hansen, J.N., Prats, H., Toudahl, K.K., Mørch Secher, N., Chan, K., Kibsgaard, J., Chorkendorff, I.: Is There Anything Better than Pt for HER? *ACS Energy Letters* **6**(4), 1175–1180 (2021) <https://doi.org/10.1021/acsenrgylett.1c00246> . Accessed 2026-01-20
- [26] Li, Z., Ge, R., Su, J., Chen, L.: Recent Progress in Low Pt Content Electrocatalysts for Hydrogen Evolution Reaction. *Advanced Materials Interfaces* **7**(14), 2000396 (2020) <https://doi.org/10.1002/admi.202000396> . Accessed 2026-01-20
- [27] Zagalskaya, A., Alexandrov, V.: Mechanistic Study of IrO₂ Dissolution during the Electrocatalytic Oxygen Evolution Reaction. *The Journal of Physical Chemistry Letters* **11**(7), 2695–2700 (2020) <https://doi.org/10.1021/acs.jpclett.0c00335> . Accessed 2026-01-20
- [28] Ping, Y., Nielsen, R.J., Goddard, W.A.: The Reaction Mechanism with Free Energy Barriers at Constant Potentials for the Oxygen Evolution Reaction at the

- IrO₂ (110) Surface. Journal of the American Chemical Society **139**(1), 149–155 (2017) <https://doi.org/10.1021/jacs.6b07557> . Accessed 2026-01-20
- [29] Kuo, D.-Y., Kawasaki, J.K., Nelson, J.N., Kloppenburg, J., Hautier, G., Shen, K.M., Schlom, D.G., Suntivich, J.: Influence of Surface Adsorption on the Oxygen Evolution Reaction on IrO₂ (110). Journal of the American Chemical Society **139**(9), 3473–3479 (2017) <https://doi.org/10.1021/jacs.6b11932> . Accessed 2026-01-20
- [30] Kresse, G., Furthmüller, J.: Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set. Physical Review B **54**(16), 11169–11186 (1996) <https://doi.org/10.1103/PhysRevB.54.11169> . Accessed 2026-01-20
- [31] Kresse, G., Furthmüller, J.: Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Computational Materials Science **6**(1), 15–50 (1996) [https://doi.org/10.1016/0927-0256\(96\)00008-0](https://doi.org/10.1016/0927-0256(96)00008-0) . Accessed 2026-01-20
- [32] Kresse, G., Hafner, J.: *Ab initio* molecular dynamics for liquid metals. Physical Review B **47**(1), 558–561 (1993) <https://doi.org/10.1103/PhysRevB.47.558> . Accessed 2026-01-20
- [33] Kresse, G., Joubert, D.: From ultrasoft pseudopotentials to the projector augmented-wave method. Physical Review B **59**(3), 1758–1775 (1999) <https://doi.org/10.1103/PhysRevB.59.1758> . Accessed 2026-01-20
- [34] Perdew, J.P., Burke, K., Ernzerhof, M.: Generalized Gradient Approximation Made Simple. Physical Review Letters **77**(18), 3865–3868 (1996) <https://doi.org/10.1103/PhysRevLett.77.3865> . Accessed 2026-01-20
- [35] Grimme, S., Antony, J., Ehrlich, S., Krieg, H.: A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. The Journal of Chemical Physics **132**(15), 154104 (2010) <https://doi.org/10.1063/1.3382344> . Accessed 2026-01-20
- [36] Hammer, B., Hansen, L.B., Nørskov, J.K.: Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals. Physical Review B **59**(11), 7413–7421 (1999) <https://doi.org/10.1103/PhysRevB.59.7413> . Accessed 2026-01-20
- [37] Silbaugh, T.L., Campbell, C.T.: Energies of Formation Reactions Measured for Adsorbates on Late Transition Metal Surfaces. The Journal of Physical Chemistry C **120**(44), 25161–25172 (2016) <https://doi.org/10.1021/acs.jpcc.6b06154> . Accessed 2026-01-20
- [38] Cheng, B.: Latent Ewald summation for machine learning of long-range interactions. npj Computational Materials **11**(1), 80 (2025) <https://doi.org/10.1038/>

s41524-025-01577-7 . Accessed 2026-01-20

- [39] Anstine, D.M., Isayev, O.: Machine Learning Interatomic Potentials and Long-Range Physics. *The Journal of Physical Chemistry A* **127**(11), 2417–2431 (2023) <https://doi.org/10.1021/acs.jpca.2c06778> . Accessed 2026-01-20
- [40] King, D.S., Kim, D., Zhong, P., Cheng, B.: Machine learning of charges and long-range interactions from energies and forces. *Nature Communications* **16**(1), 8763 (2025) <https://doi.org/10.1038/s41467-025-63852-x> . Accessed 2026-01-20
- [41] Kim, D., Wang, X., Zhong, P., King, D.S., Inizan, T.J., Cheng, B.: A universal augmentation framework for long-range electrostatics in machine learning interatomic potentials. *arXiv*. Version Number: 1 (2025). <https://doi.org/10.48550/ARXIV.2507.14302> . <https://arxiv.org/abs/2507.14302> Accessed 2026-01-20
- [42] Chen, D., Shang, C., Liu, Z.-P.: Automated search for optimal surface phases (ASOPs) in grand canonical ensemble powered by machine learning. *The Journal of Chemical Physics* **156**(9), 094104 (2022) <https://doi.org/10.1063/5.0084545> . Accessed 2026-01-20
- [43] Sun, M., Jin, B., Yang, X., Xu, S.: A Machine-Learning Accelerated Grand Canonical Sampling Framework for Nuclear Quantum Effects in Constant Potential Electrochemistry. *arXiv*. Version Number: 3 (2024). <https://doi.org/10.48550/ARXIV.2407.12458> . <https://arxiv.org/abs/2407.12458> Accessed 2026-01-20
- [44] Jinnouchi, R.: Grand-Canonical First Principles-Based Calculations of Electrochemical Reactions. *Journal of The Electrochemical Society* **171**(9), 096502 (2024) <https://doi.org/10.1149/1945-7111/ad7326> . Accessed 2026-01-20
- [45] Chen, X., El Khatib, M., Lindgren, P., Willard, A., Medford, A.J., Peterson, A.A.: Atomistic learning in the electronically grand-canonical ensemble. *npj Computational Materials* **9**(1), 73 (2023) <https://doi.org/10.1038/s41524-023-01007-6> . Accessed 2026-01-20

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- [si3.pdf](#)