Supplementary Information: Evaluating the Transfer Learning from Metals to Oxides with GAME-Net-Ox

Thomas Van Hout,[a,b] Oliver Loveday,[a,c] Jordi Morales-Vidal,[a] Santiago Morandi,[a] and Núria López*[,a]

[a] *Institute of Chemical Research of Catalonia, The Barcelona Institute of Science and Technology (ICIQ-CERCA), Av. Països Catalans 16, 43007, Tarragona, Spain.*

[b] *Eindhoven University of Technology, Den Dolech 25612 AZ Eindhoven, The Netherlands.*

[c] *Department of Physical and Inorganic Chemistry, Universitat Rovira i Virgili, Campus Sescelades, N4 Block, C. Marcel·lí Domingo 1, 43007, Tarragona, Spain.*

* *Corresponding author. E-mail: nlopez@iciq.es*

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S1. SUPPLEMENTARY FIGURES

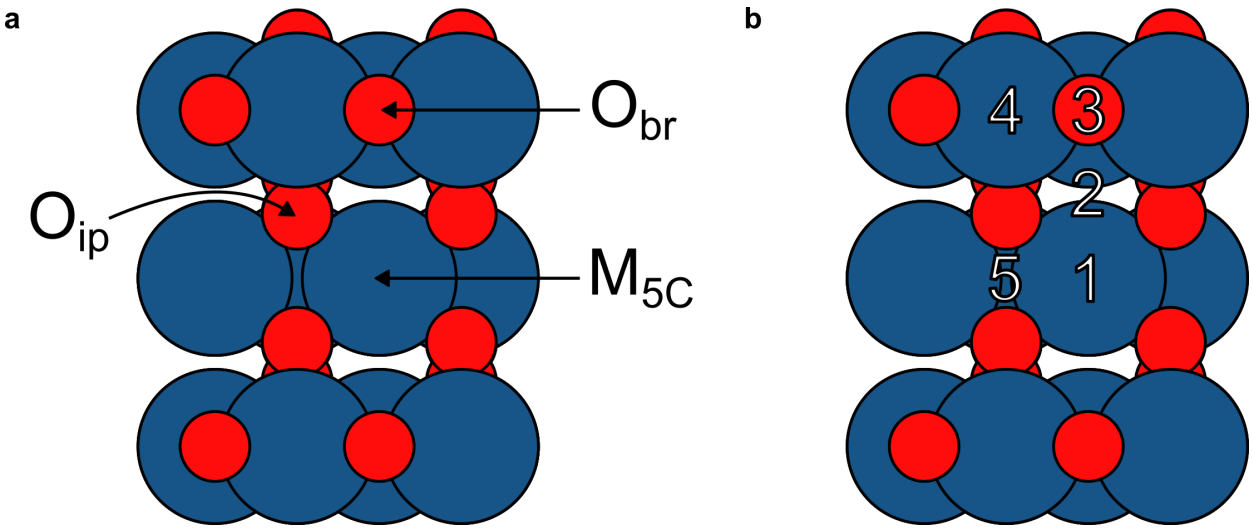

FIG. S1: Rutile (110) surfaces and adsorption sites, r-MO_2 surface top view. **a** Type of surface atoms: M_{5C}: 5-coordinated metal, O_{br}: Bridge Oxygen, O_{ip}: In-plane Oxygen. **b** Considered sites for initial adsorbate placement: (1) Top M_{5C} site, (2) Hollow M_{5C}-O_{br} site, (3) Top O_{br} site, (4) Bridge O_{br} site, and (5) Hollow M_{5C}-O_{ip} site.

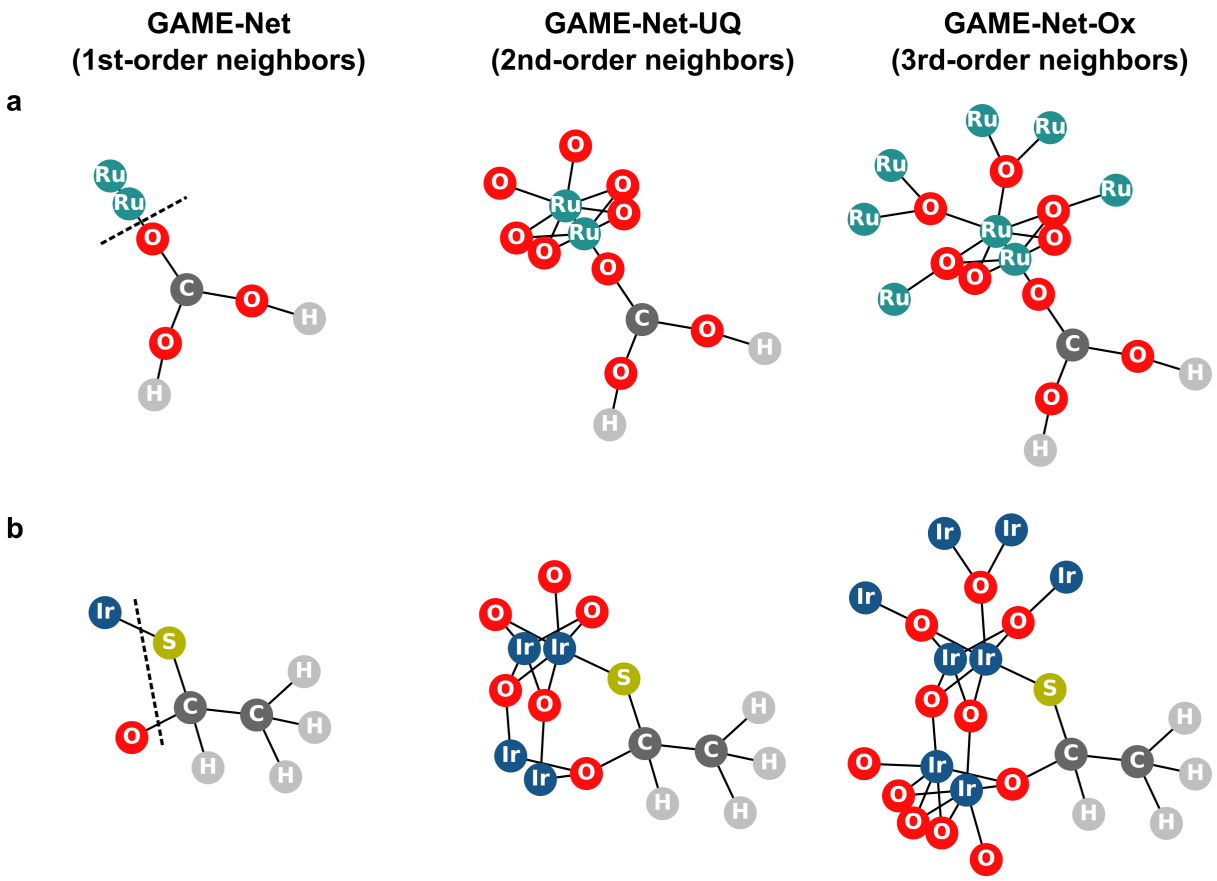

FIG. S2: Example of graph representations for **a** carbonic acid CH_2O_3 on $RuO_2(110)$ and **b** ethanethial C_2H_4S on $IrO_2(110)$ adsorption structures, as function of the surface neighbor order with respect to the adsorbate. GAME-Net-Ox employs the most extended surface representation, which includes the 3rd order neighbors and the coordination number (CN). Note that the graph representation employed by GAME-Net is not suitable to retrieve the composition of the oxide surface.

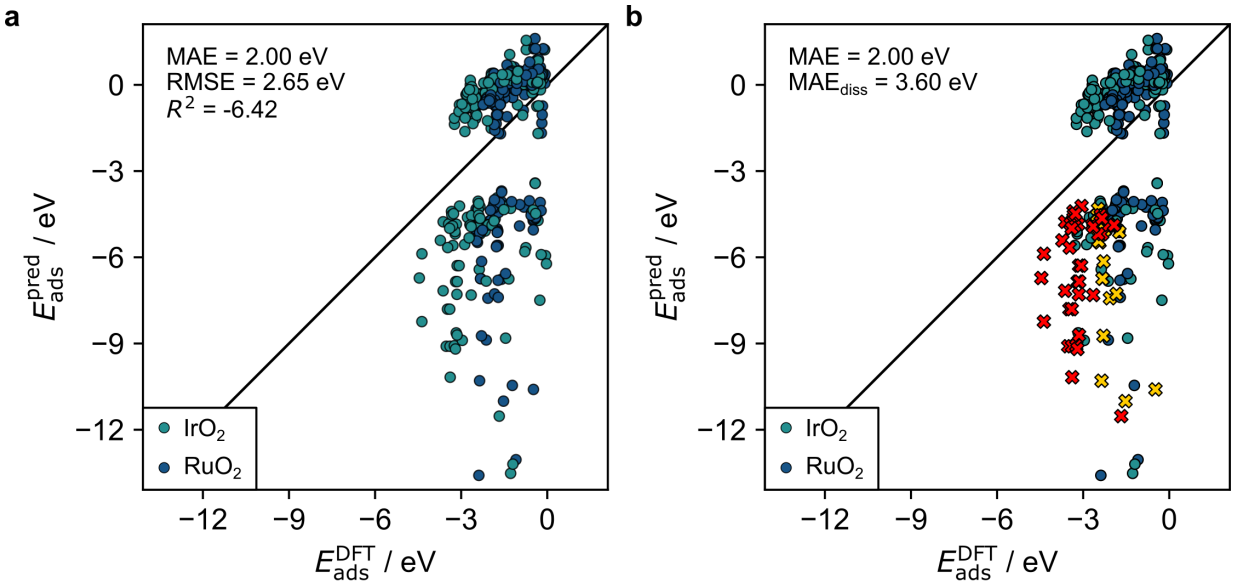

FIG. S3: Parity plots of GAME-Net predicted, *vs.* DFT adsorption energies on conductive oxides (IrO_2 and RuO_2, n=536). **a** All adsorption configurations. **b** The same data with proton-dissociation events highlighted as crosses for IrO_2 (red) and RuO_2 (yellow).

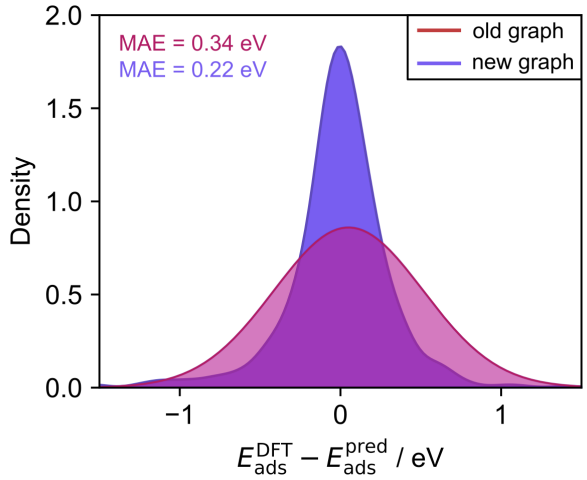

FIG. S4: Distribution of prediction errors and associated MAE when using the original GAME-Net graph representation (red) and when including the coordination number (CN) and the 3^{rd} order neighbors for the surface atoms (blue) for the model trained on conductive IrO_2 and RuO_2 metal oxides.

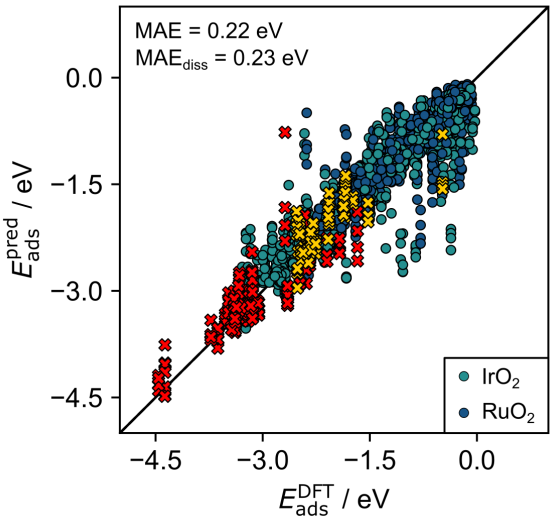

FIG. S5: Parity plot of predicted *vs.* DFT adsorption energies for GAME-Net-Ox on conductive oxides (IrO_2, RuO_2). Cross-shaped points correspond to proton-dissociations for IrO_2 (red) and RuO_2 (yellow) (n=2096).

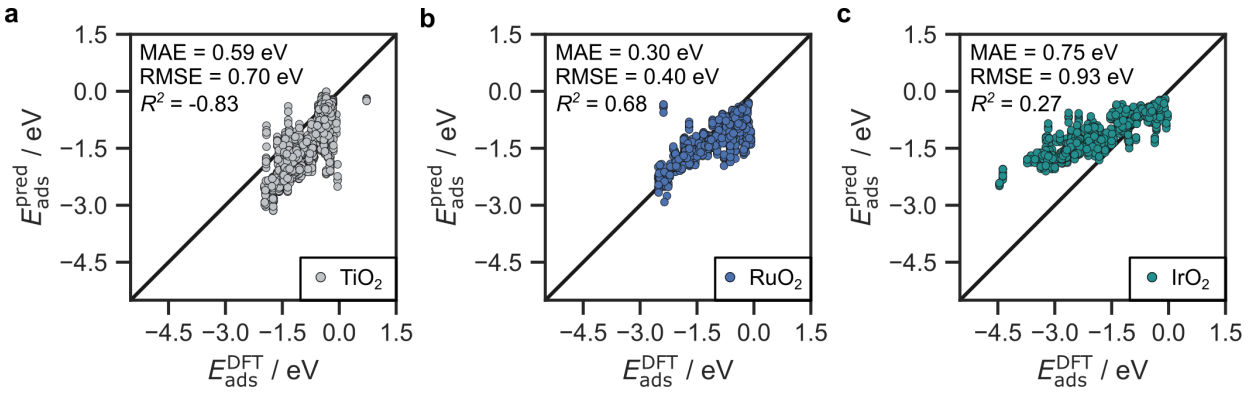

FIG. S6: Parity plots evaluating model metal oxide generalization. The tests show the model: **a** trained on IrO_2 and RuO_2 and tested on TiO_2 (n=1680), **b** trained on IrO_2 and TiO_2 and tested on RuO_2 (n=1350), and **c** trained on RuO_2 and TiO_2 and tested on IrO_2 (n=1270).

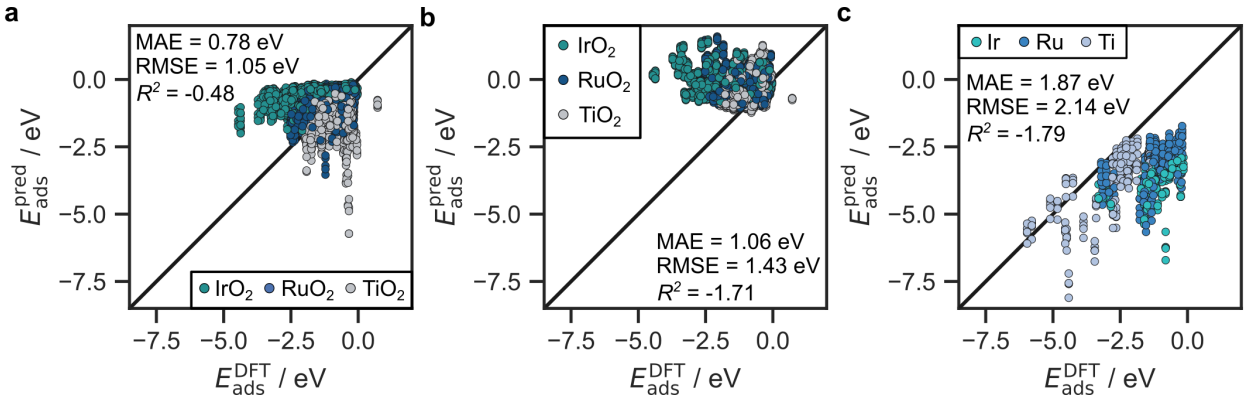

FIG. S7: Parity plots evaluating model transferability between metal and oxide domains. The tests show the model: **a** trained on all metals and tested on all oxides (n=4300); **b** trained on a metal subset (Ir, Ru, Ti) and tested on all oxides (n=4300), and **c** trained on all oxides and tested on the metal subset (n=540).

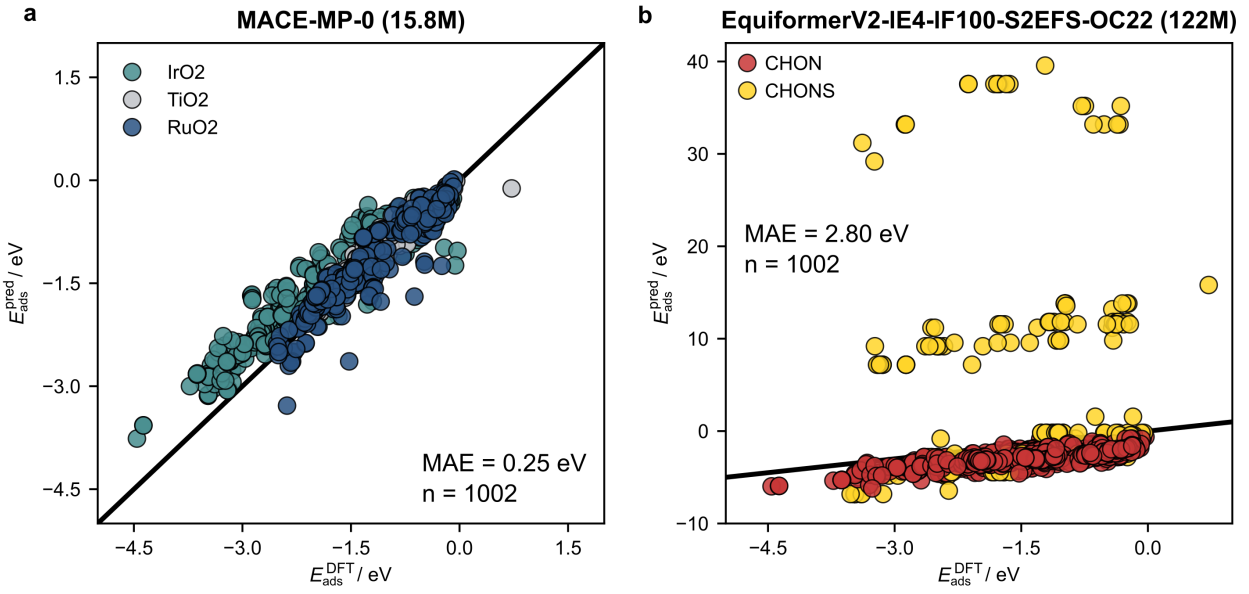

FIG. S8: Performance of **a** MACE-MP-0 and **b** EquiformerV2-OC22 in predicting the DFT adsorption energy starting from the DFT-relaxed structures. Points in panel **b** are colored based on the presence of S in the adsorbate.

S2. SUPPLEMENTARY TABLES

TABLE S1: List of adsorbates included in the dataset, grouped by adsorbate family.

Molecule	**Formula**
C_xH_y	
Methane	CH_4
Ethane	C_2H_6
Propane	C_3H_8
Ethene	C_2H_4
Propylene	C_3H_6
Acetylene	C_2H_2
Prop-1-yne	C_3H_4
C_xH_yO	
Methanol	CH_3OH
Ethanol	C_2H_5OH
Propan-2-ol	C_3H_7OH
Formaldehyde	CH_2O
Acetaldehyde	C_2H_4O
Propan-2-one	C_3H_6O
Methoxymethane	CH_3OCH_3
C_xH_yS	
Methanethiol	CH_3SH
Methanethial	CH_2S
Ethanethiol	C_2H_5SH
Ethanethial	C_2H_4S
Propane-2-thiol	C_3H_7SH
Propane-2-thione	C_3H_6S
Dimethylsulfane	CH_3SCH_3

Molecule	**Formula**
Amines	
Methanamine	CH_3NH_2
Ethanamine	$C_2H_5NH_2$
Propan-2-amine	$C_3H_7NH_2$
Trimethylamine	$(CH_3)_3N$
Imines	
Methanimine	CH_2NH
Ethanimine	C_2H_3NH
Propan-2-imine	C_3H_5NH
N-methylmethanimine	$CH_3N{=}CH_2$
$C_xH_yO_{n=(2,3)}$	
Carbonic acid	H_2CO_3
Formic acid	$HCOOH$
Acetic acid	CH_3COOH
Carbamate esters	
Carbamic acid	NH_2COOH
Amides	
Formamide	$HCONH_2$
Acetamide	CH_3CONH_2
Oximes	
Formaldoxime	CH_2NOH
Amidines	
Formimidamide	$HN{=}CHNH_2$
Acetimidamide	$CH_3N{=}CHNH_2$

TABLE S2: Statistics related to the DFT structures → graph post-filtering process for isomorphic graphs. Values obtained with the conversion parameters defined in the Manuscript.

Material	**DFT relaxations**	**Unique graphs**	**Filtered graphs**	**Conversion** [%]
RuO_2	302	270	32	89.4
IrO_2	313	254	59	81.2
TiO_2	387	336	51	86.8
Total	1002	860	142	85.8

TABLE S3: GAME-Net-Ox architecture and number of parameters for each internal layer. Table obtained with `torchinfo` Python package. PMA=Pooling by Multi-head Attention; MAB=Multi-head Attention Block.

Layer(type)	**Sub-layer Parameters**
Linear	3,360
SAGEConv(1) MeanAggregation	
Linear	25,600
Linear	25,600
SAGEConv(2) MeanAggregation	
Linear	25,600
Linear	25,600
SAGEConv(3) MeanAggregation	
Linear	25,600
Linear	25,600
TAGConv SumAggregation	
Linear	25,600
Linear	25,600
Linear	25,600
Linear	25,600
Linear	25,600
Linear	320
PMA	160
MAB Linear	25,600
Linear	25,600
Linear	25,600
Linear	25,600
Total	387,840

TABLE S4: GAME-Net architecture and number of parameters for each internal layer. Table obtained with `torchinfo` Python package. The `GraphMultisetTransformer` pooling layer relies on Pytorch Geometric 2.0.3. PMA=Pooling by Multi-head Attention.

Layer(type)	**Sub-layer Parameters**
Linear	3,040
SAGEConv(1)	
Linear	25,600
Linear	25,600
SAGEConv(2)	
Linear	25,600
Linear	25,600
SAGEConv(3)	
Linear	25,600
Linear	25,600
GraphMulstisetTransformer	
Linear	25,760
Linear	161
PMA	103,200
Total	285,761

TABLE S5: Game-Net-UQ architecture and number of parameters for each internal layer. Table obtained with `torchinfo` Python package. Due to breaking changes after Pytorch Geometric 2.0.3, the `GraphMultisetTransformer` pooling layer has been implemented manually by the authors. PMA=Pooling by Multi-head Attention; MAB=Multi-head Attention Block.

Layer(type)	**Sub-layer Parameters**
Linear	3,840
SAGEConv(1) MeanAggregation	
Linear	36,864
Linear	36,864
SAGEConv(2) MeanAggregation	
Linear	36,864
Linear	36,864
SAGEConv(3) MeanAggregation	
Linear	36,864
Linear	36,864
TAGConv SumAggregation	
Linear	36,864
Linear	36,864
Linear	36,864
Linear	36,864
Linear	36,864
Linear	384
PMA	192
MAB Linear	36,864
Linear	36,864
Linear	36,864
Linear	36,864
Total	557,376

TABLE S6: Dissociative adsorptions included in the dataset, grouped by family and surface of dissociation.

Molecule	**Formula**	**Surface**
C_xH_y		
Prop-1-yne	C_3H_4	RuO_2
C_xH_yO		
Acetaldehyde	C_2H_4O	IrO_2
Ethanol	C_2H_5OH	IrO_2
Methanol	CH_3OH	IrO_2
C_xH_yS		
Ethanethiol	C_2H_5SH	IrO_2, RuO_2
Methanethiol	CH_3SH	IrO_2, RuO_2
Propane-2-thiol	C_3H_7SH	IrO_2, RuO_2
Propane-2-thione	C_3H_6S	IrO_2
Imines		
N-methylmethanimine	$CH_3N{=}CH_2$	IrO_2
$C_xH_yO_{n=(2,3)}$		
Acetic acid	CH_3COOH	IrO2, RuO_2
Carbonic acid	H_2CO_3	IrO_2, RuO_2
Formic acid	$HCOOH$	IrO_2, RuO_2
Carbamate esters		
Carbamic acid	NH_2COOH	IrO_2, RuO_2
Amides		
Acetamide	CH_3CONH_2	IrO_2
Formamide	$HCONH_2$	IrO_2, RuO_2
Oximes		
Formaldoxime	CH_2NOH	IrO_2, RuO_2
Amidines		
Acetimidamide	$CH_3N{=}CHNH_2$	IrO_2
Formimidamide	$HN{=}CHNH_2$	IrO_2

TABLE S7: Performance of MACE-MP-0 and EquiformerV2-122M ML interatomic potentials (MLIPs) on predicting the DFT adsorption energy on rutile oxides. The EquiformerV2 model checkpoint is named `EquiformerV2-lE4-lF100-S2EFS-OC22`, and included in the FairChem-V1 GitHub repository. Mean Absolute Error (MAE) values are in eV. MAE_{RS} refers to the MLIP predictions obtained by running a single-point on the DFT-relaxed structures (VASP CONTCAR file). $\mathbf{n}^*$ and $\mathbf{MAE}^*_{\mathbf{RS}}$ neglect adsorption structures with S-containing adsorbates as Equiformer has not been trained with these systems.

	MACE-MP-0 (15.8M)		**EquiformerV2-122M (OC22)**			
Material	**n**	$\mathbf{MAE_{RS}}$	**n**	$\mathbf{MAE_{RS}}$	$\mathbf{n}^*$	$\mathbf{MAE^*_{RS}}$
$RuO_2(110)$	302	0.18	302	3.22	246	1.53
$IrO_2(110)$	313	0.46	313	3.51	249	1.46
$TiO_2(110)$	387	0.14	387	1.91	314	1.22
Total	1002	0.25	1002	2.80	809	1.39