

# Supplementary Information for Adsorbed O Promotes Alternative, Nonselective Oxametallacycle Reaction Pathways in Ag-Catalyzed Epoxidation

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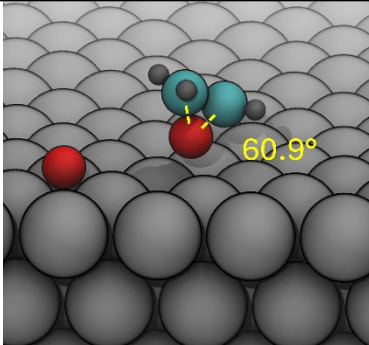
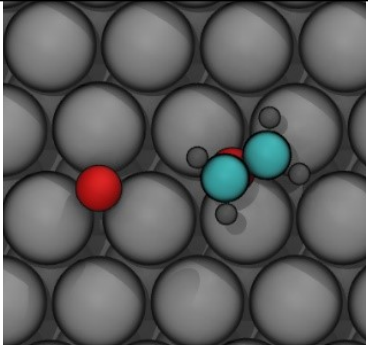
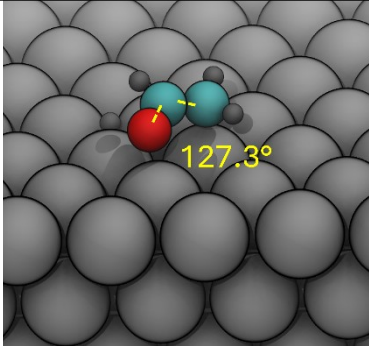
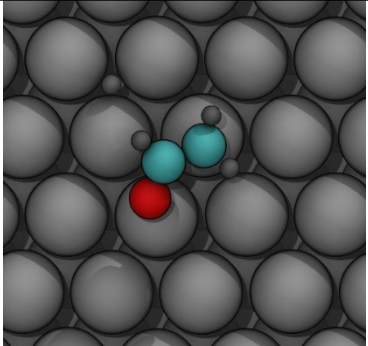
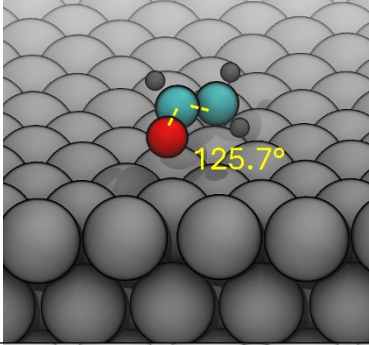
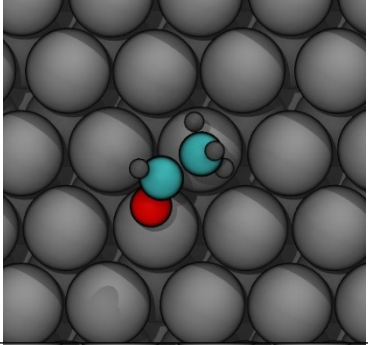
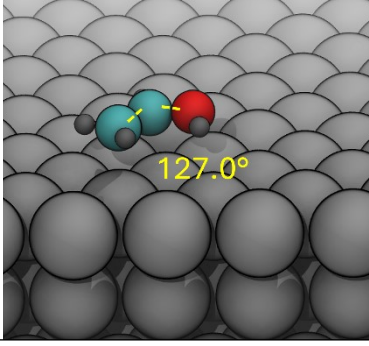
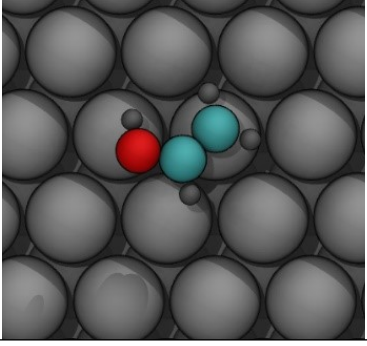
<sup>†</sup>These two authors contributed equally to this work

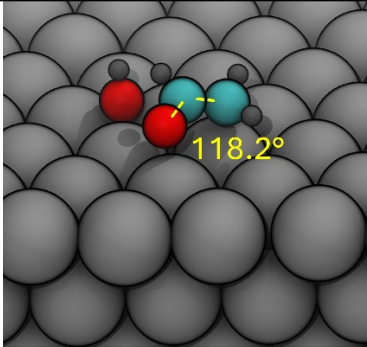
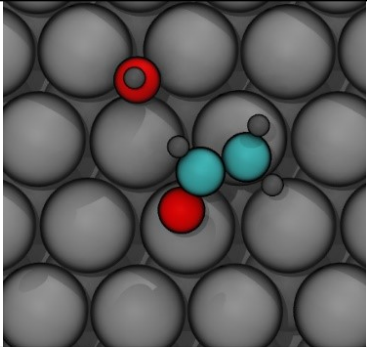
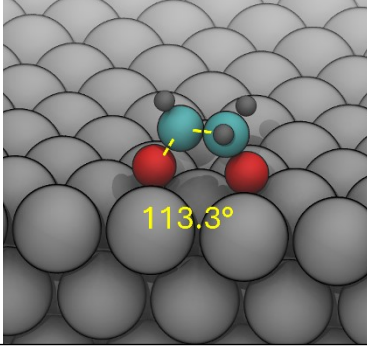
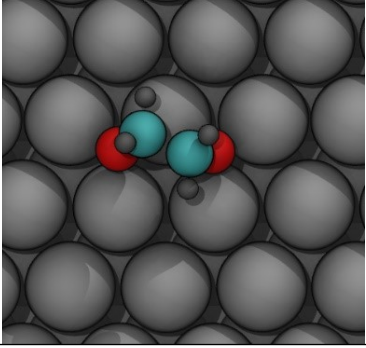
## 1 Adsorbate configurations

The bond angles and adsorption sites for Figure 1 are shown in Table S1.

**Table S1:** The adsorbates used in Figure 1. OMC and EO with surface O present are shown, as they have the same angle and site of the same case without surface O.

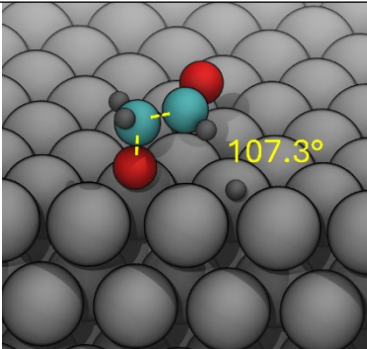
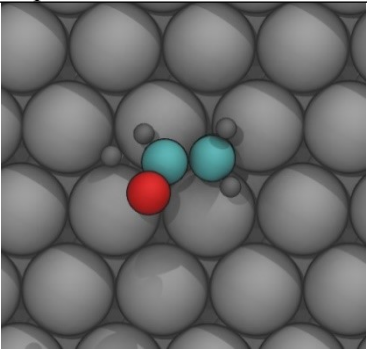
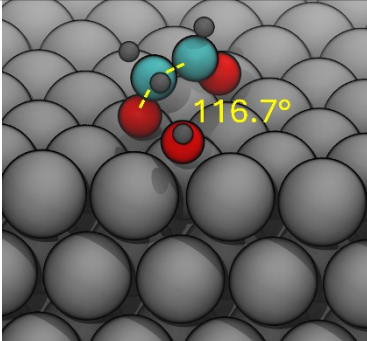
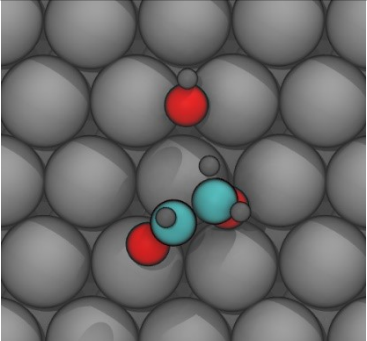
Adsorbate (from OMC)	Side view	Top view
OMC		
OMC with surface O		

EO with surface O		
$H_{\text{surf}}$		
AA		
VA		

$\text{OH}_{\text{surf}}$		
EDO		

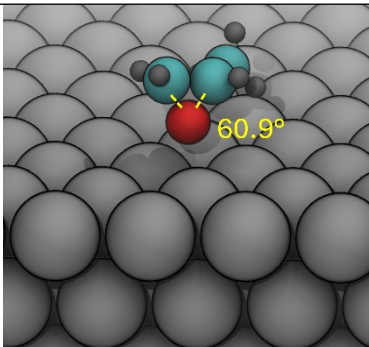
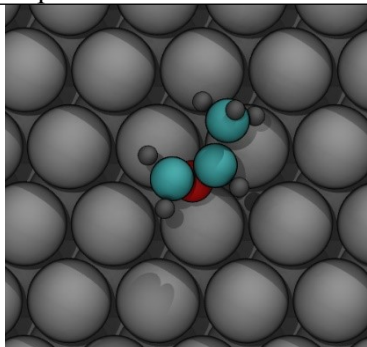
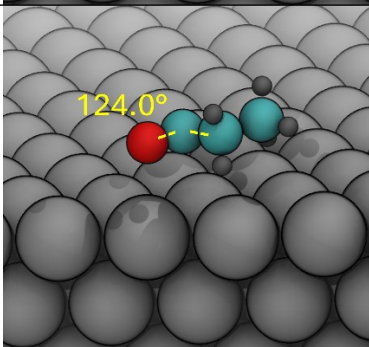
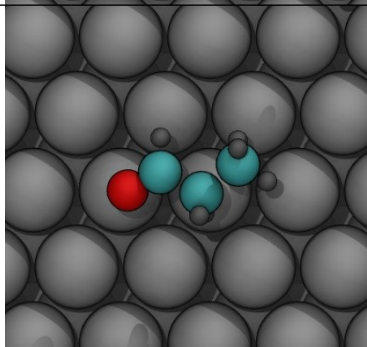
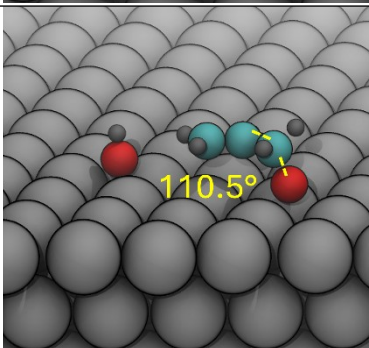
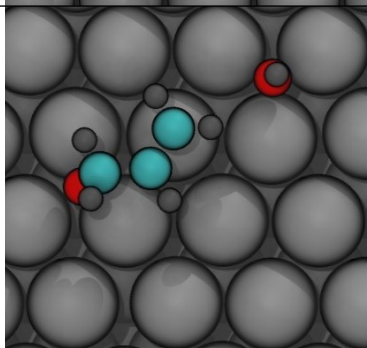
The bond angles and adsorption sites for Figure 4 are shown in Table S2.

**Table S2:** Additional structures relevant to Figure 4. EO and AA were shown in Table S1.

Adsorbate (from EDO)	Side view	Top view
$\text{H}_{\text{surf}}$		
$\text{OH}_{\text{surf}}$		

The bond angles and adsorption sites for Figure 5 are shown in Table S3.

**Table S3:** The adsorbates from Figure 5 showing the PO pathway.

Adsorbate (OMC)	Side view	Top view
PO		
PA		
OH <sub>surf</sub>		
PDO	