

## FINAL PROJECT REPORT

Project Title: Experimental and Theoretical Studies of Surface Oxametallacycles:  
Connections to Heterogeneous Olefin Epoxidation

Award No.: DE-FG02-84ER13290

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### ABSTRACT:

This project has aimed at the rational design of catalysts for direct epoxidation of olefins. This chemistry remains one of the most challenging problems in heterogeneous catalysis. Although the epoxidation of ethylene by silver catalysts to form ethylene oxide (EO) has been practiced for decades, little progress has been made in expanding this technology to other products and processes. We have made significant advances through the combination of surface science experiments, Density Functional Theory (DFT) calculations, and catalytic reactor experiments, toward understanding the mechanism of this reaction on silver catalysts, and to the rational improvement of selectivity. The key has been our demonstration of surface oxametallacycle intermediates as the species that control reaction selectivity. This discovery permits the influence of catalyst promoters on selectivity to be probed, and new catalyst formulations to be developed. It also guides the development of new chemistry with potential for direct epoxidation of more complex olefins.

During the award period we have focused on 1. the formation and reaction selectivity of complex olefin epoxides on silver surfaces, and 2. the influence of co-adsorbed oxygen atoms on the reactions of surface oxametallacycles on silver, and 3. the computational prediction, synthesis, characterization and experimental evaluation of bimetallic catalysts for ethylene epoxidation. The significance of these research thrusts is as follows. Selective epoxidation of olefins more complex than ethylene requires suppression of not only side reactions available to the olefin such as C-H bond breaking, but it requires formation and selective ring closure of the corresponding oxametallacycle intermediates.

Our combined experimental and theoretical studies have shown that epoxides containing C=C bonds, including epoxybutene, styrene oxide, and isoprene oxide, undergo activated ring-opening on Ag(110) and (111) surfaces to form stable oxametallacycles. The stability of these intermediates is increased in each case by interaction of the unsaturated substituent with surface metal atoms. All three oxametallacycles react by ring closure to form the parent epoxides, as well as undergoing isomerization to produce the corresponding unsaturated aldehyde isomers. These results demonstrate a feasible pathway for epoxidation of complex olefins, including those like isoprene that contain reactive allylic hydrogens.

The second thrust has explored the effect of oxygen on oxametallacycle surface chemistry. While our representation of the surfaces of silver catalysts as oxygen-free has been remarkably successful in leading to design of new bimetallic catalysts, others have contended that oxygen must be present on the surface and must be accounted for in any quantitative model. We have completed studies of the interaction of oxametallacycles derived from ethylene oxide with oxygen at various concentrations on Ag(110) and (111) surfaces. These results show that oxygen has relatively little influence on the formation, stability, or selectivity of oxametallacycles; rather, its principal role in side reactions appears to be to intercept and oxidize acetaldehyde via formation of surface acetate intermediates. By varying the surface oxygen coverage prior to EO ring opening, we can trace out each of the steps in our microkinetic model of the catalytic process, including EO formation, acetaldehyde formation, acetaldehyde oxidation, and acetate oxidation. Many of these steps have been observed individually before, but not in the sequence in which they occur in temperature programmed reaction experiments.

In the third thrust, including complementary studies funded by grant FG02-03ER15468 (see publication list), we have constructed micro-kinetic models that allow us to assess the performance of multi-component catalysts based on DFT results for binding of all adsorbates, rather than focusing solely on the oxametallacycle reaction steps. These require extensive computations for input. Our demonstration of the importance of combining DFT and microkinetic modeling to make *accurate* predictions of catalyst performance is one of the most important outcomes of this work. Extensive catalyst characterization studies have helped to understand cases in which the DFT calculations did not lead to useful predictions because the state of the catalyst was not well represented by the model.

#### **DOE INTEREST:**

Selectivity gains in partial oxidation catalysis translate into direct savings of hydrocarbon raw materials and reduction of CO<sub>2</sub> production. For example, annual CO<sub>2</sub> production from unselective reactions in ethylene epoxidation alone amounts to nearly 1 million tons! Our work represents one of the first examples of catalyst design for improved selectivity based on first principles approaches.

## RESEARCH ACCOMPLISHMENTS

### *Research Goals*

This research has combined DFT calculations and surface science experiments as the principal tools for understanding oxametallacycle chemistry and epoxidation catalysis, as well as promoter and alloy effects at the molecular level. These results can then be integrated into microkinetic models whose predictions can be benchmarked against experimental results for heterogeneous epoxidation catalysts. The ultimate goal of this work is to develop a level of understanding of this process that will permit quantitative prediction of catalyst performance, including that of novel catalysts such as the bimetallics that we have advanced. In doing so, we aim to develop a framework for catalyst design for epoxidation of larger olefins, including propylene and styrene, and to demonstrate paradigms for catalyst design from first principles.

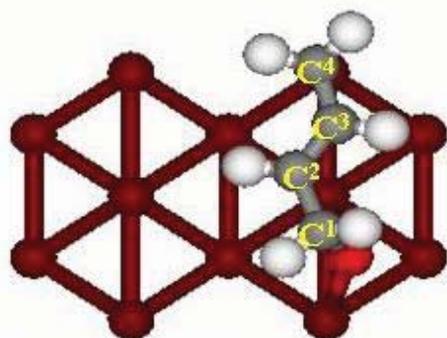
### *Description of Research Effort*

During the award period we have focused on three principal research areas: experimental and computational studies of complex oxametallacycles on silver surfaces; reactions of oxametallacycles in the presence of co-adsorbed oxygen atoms; and the computational prediction, synthesis, characterization and experimental evaluation of bimetallic catalysts for ethylene epoxidation. These are described below.

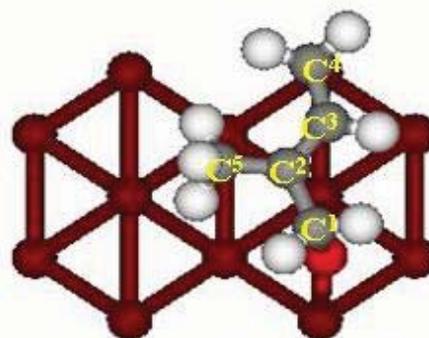
Our **fundamental surface science and DFT studies of the epoxides of conjugated olefins** have focused on the oxides of butadiene, styrene, and isoprene. For each of these molecules we have identified oxametallacycles as the reactive intermediates on the crystal surface. TPD experiments have shown that each of these epoxides gives rise to more a stable oxametallacycle than does EO. In the case of styrene oxide (StO) on both Ag(111) and (110) surfaces, the oxametallacycle was observed to reform styrene oxide along with phenylacetaldehyde at ca. 485 K. These products, combined with HREELS and HRXPS results, indicate the preservation of the phenyl substituent and confirm theoretical predictions regarding the stability of these intermediates.

Most recently we have extended this chemistry to isoprene oxide (IO), forming the first stable oxametallacycle containing allylic hydrogens. This is an important step toward accomplishing direct selective epoxidation of propylene with silver-based catalysts. Isoprene oxide (2-methyl-2-vinyl oxirane) forms a strongly bound oxametallacycle intermediate on the Ag(110) surface. The oxametallacycle undergoes ring-closure to reform isoprene oxide in two peaks at 320 and 460 K during reaction subsequent to epoxide adsorption at low Ag(110) surface temperatures, while epoxide doses at higher surface temperatures lead to isomerization of the oxametallacycle and desorption of the aldehyde isomer, 2-methyl-2-butenal, in a single peak at 460 K; isomerization occurs via 1,4-hydrogen transfer in the oxametallacycle species. Isoprene oxide ring opens at the carbon bound to the unsaturated vinyl and allylic methyl substituent groups to form an

oxametallacycle on the Ag(110) surface. The structure of the isoprene oxide-derived oxametallacycle resembles that formed from ring-opening the non-allylic counterpart, epoxybutene (EpB) on Ag(110). The calculated structures of the oxametallacycles derived from isoprene oxide and EpB are shown below. DFT results indicate that the methyl group in the isoprene oxide derive structure is only slightly destabilizing, reducing the energy of the ring opening reaction by only 2 kcal/mol relative to that for EpB.

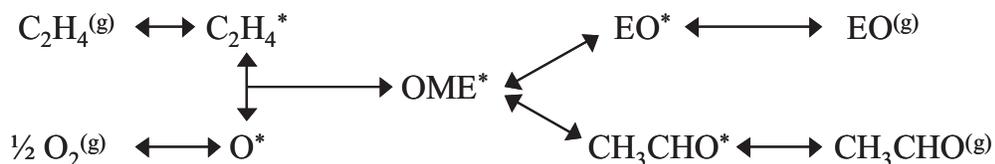


DFT predicted EpB OME Ag<sub>12</sub>(110)



DFT predicted IO OME Ag<sub>12</sub>(110)

Throughout our studies of the mechanism of olefin epoxidation, we have constructed microkinetic models containing increasing numbers of steps in order to predict new catalyst formulations (e.g., bimetallics) and to account for the performance of catalysts operating under steady-state reaction conditions. As we have demonstrated previously, simply considering the branching reactions of surface oxametallacycles is sufficient to predict (correctly) that Cu-Ag bimetallics should be more selective than silver catalysts for ethylene epoxidation. We have carried out extensive DFT calculations to scout for other promising bimetallic combinations. As detailed in publication #5 below, while bimetallic combinations such as Pd-Ag and Pt-Ag appear favorable if one considers the oxametallacycle branching reactions to be *irreversible*, their advantage disappears if one recognizes that the interconversion of oxametallacycles and ethylene oxide is *reversible*, and low barriers to this process disfavor selectivity because they favor product readsorption and isomerization. We have proposed a more extensive microkinetic model based on the reaction network below to incorporate these factors.



This network takes into account the reaction of ethylene with adsorbed oxygen, but it does not explicitly account for possible reactions of oxygen with the species “downstream” in the reaction network: the oxametallacycle (OME), adsorbed ethylene oxide, and adsorbed acetaldehyde. It is well known from the surface science studies of Madix and co-workers that adsorbed oxygen will oxidize acetaldehyde to surface acetates on silver. Moreover, reaction of oxygen atoms with these acetates occurs at much lower temperatures than the thermal decomposition of acetates in an oxygen-free environment. The possibility that similar reactions might occur with surface oxametallacycles or EO had not previously been explored, however.

We have completed **studies of the reactions of EO on oxygen-containing Ag(110) and (111) surfaces**. We find that EO still undergoes ring opening and closing reactions with relatively little variation in kinetics or selectivity when oxygen is present. This helps to explain the success of our simple models of the epoxidation mechanism that have neglected possible surface oxygen effects. However, by varying the EO/O ratio on the surface we are able to observe each of the key steps in the combustion pathway in TPD experiments. At low EO/O ratios, acetaldehyde formed by oxametallacycle isomerization is oxidized to acetates which undergo further oxidation by excess oxygen near 400K. As the initial EO/O ratio is increased, less oxygen remains after acetate formation, and peaks corresponding to acetate pyrolysis grow in at ~600K at the expense of the acetate oxidation peaks at lower temperature. At intermediate EO/O ratios, it is possible to observe all of the product reaction channels in a single TPD experiment: EO formation at ~300K, acetate oxidation at ~400K, and acetate pyrolysis at ~600K. This observation provides important support for microkinetic modeling efforts, since it shows that the evolution of selective and non-selective products is controlled by continuously varying competition between reaction pathways and not by abrupt transitions that might arise from surface reconstructions or phase transformations at different oxygen concentrations.

Table 1 summarizes the product distributions from the TPD spectra obtained following adsorption of different exposures of ethylene oxide at 250 K on the clean Ag(110) surface. Oxametallacycle surface coverages ( $\theta_{\text{OME}}$ ), reported in monolayers (ML), were calibrated against the saturated TPD trace for desorption of oxygen from Ag(110) at 570 K (not shown). The oxygen TPD peak saturates at a coverage of 0.5 ML. The total coverage of oxametallacycles on the surface was equated with the sum of yields of C<sub>2</sub>-containing products.

Table 1: Product distribution (monolayers, ML) from TPD of ethylene oxide adsorbed at 250 K on clean Ag(110).

EO Dose (L)	Coverage (ML)	Yields				EO
		$\theta_{\text{OME}}$	$Y_{\text{EO}}$	$Y_{\text{AcA}}$	$Y_{\text{Et}}$	$Y_{\text{EtOH}}$
0.5L	0.26	0.18	0.08	0.00	0.00	69
1L	0.37	0.25	0.12	0.00	0.00	68
5L	0.39	0.26	0.13	0.00	0.00	67
10L	0.45	0.29	0.16	0.00	0.00	64

Increasing the oxametallacycle coverage on the Ag(110) surface decreased the selectivity to ethylene oxide only slightly. The selectivity to ethylene oxide decreased from 69 to 64% as the oxametallacycle coverage increased from 0.26 to 0.45 ML; the oxametallacycle coverage saturated at ca. 0.5 ML on the clean Ag(110) surface. Oxametallacycles formed from ring-opening styrene oxide on Ag(110) exhibited a similar trend, with decreasing selectivity to the epoxide as the oxametallacycle coverage increased. The ethylene oxide yield ( $Y_{EO}$ ) increased with coverage as the increasing oxametallacycle coverage ( $\theta_{OME}$ ) more than compensated for the apparent selectivity decrease.

Table 2 summarizes the product distribution following ethylene oxide adsorption on the O-covered Ag(110) surface, as well as the amount of unreacted oxygen that desorbed during TPD. The selectivities to ethylene oxide were ca. 10 to 20% lower on the O-covered surface than on the clean Ag(110) surface throughout the range of coverages explored.

Table 2: Product distribution (monolayers, ML) from TPD of ethylene oxide adsorbed at 250 K on oxygen-covered Ag(110).

EO Dose (L)	Coverage (ML)		Yields					EO Selectivity
	$\theta_{O,Unreacted}$	$\theta_{OME}$	$Y_{CO_2}$	$Y_{EO}$	$Y_{AcA}$	$Y_{Et}$	$Y_{EtOH}$	S(%)
0.1L	0.50	0.14	0.02	0.08	0.00	0.03	0.01	62
0.5L	0.40	0.23	0.07	0.10	0.00	0.03	0.03	53
5L	0.16	0.40	0.04	0.20	0.00	0.11	0.05	53
10L	0.17	0.70	0.11	0.24	0.00	0.17	0.18	38

At the highest oxametallacycle coverages, the yield of ethylene oxide was approximately 20% lower on the oxygen-covered surface than on the clean surface, although the oxametallacycle coverage was approximately 40% higher on this surface. No acetaldehyde desorption was observed from the O-covered surface. Instead, the principal side products were ethylene and  $CO_2$ .

The presence of coadsorbed oxygen on Ag(110) may increased the capacity of the surface for oxametallacycles. The activation barrier for oxametallacycle ring-closure, however, was not affected by the presence of oxygen, as ethylene oxide was produced at the same temperatures on both the O-covered and clean Ag(110) surface. Previous DFT calculations by Bocquet et al. also showed that the activation barrier for oxametallacycle ring-closure on Ag(111) was not significantly changed by the presence of co-adsorbed oxygen.

The principal impact of coadsorbed oxygen on the selectivity of oxametallacycle conversion to ethylene oxide appears to be the promotion of the reverse reaction from the oxametallacycle to ethylene and oxygen, rather than perturbation of the ring-closure/isomerization reaction rates. Our observation of ethylene production from

ethylene oxide on the O-covered surface, but not on the clean surface, suggests that the presence of oxygen must also reduce the barrier to ethylene release from the oxametallacycle. While oxygen also increases the heat of adsorption of ethylene oxide and acetaldehyde on Ag(110) and Ag(111) surfaces, there is little evidence for alteration of the activation barriers for the formation of these products from oxametallacycles, either from our TPD results, or from previous DFT calculations. Indeed, if one omits ethylene from the determination of oxametallacycle reaction selectivities, the fraction of oxametallacycles reacted to ethylene oxide relative to the total reacting to oxygen-containing products is essentially the same on both the clean and O-covered surfaces. This is consistent with the conclusion that ethylene oxide selectivity is controlled by competing reactions of the oxametallacycle, and that CO<sub>2</sub> is formed by combustion of acetaldehyde produced from the oxametallacycle. The results of the present study provide no evidence for oxygen attack on ethylene oxide or on the oxametallacycle. The kinetics and selectivity of CO<sub>2</sub> formation can be accounted for entirely by the secondary reactions of the acetaldehyde product.

Figure 1 illustrates the effect of oxygen on the reaction coordinate in schematic form. As noted above, the comparable peak temperatures for oxametallacycle reaction on Ag(111), Ag(110), and O-Ag(110) surfaces, along with DFT calculations, suggest that the heat of reaction to form this species from gas phase ethylene oxide is insensitive to surface structure and oxygen content. Therefore, one can assess shifts in barrier heights and adsorbed states relative to the oxametallacycle. Activation energy values for both Ag(111) and Ag(110) surfaces are included in Figure 1 since a complete set is not available for either surface in the literature. However, the observed insensitivity to surface structure in both single crystal and DFT results suggests that equating the two surfaces is a reasonable approximation in trying to understand the effects of coadsorbed oxygen on reactions on either surface.

The key point illustrated in Figure 1 is that, while the “forward” reactions of the oxametallacycle are not affected significantly by the presence of oxygen, the “reverse” reaction to ethylene plus oxygen is affected. In order for the barriers for ethylene, ethylene oxide, and acetaldehyde reactions to become comparable, the barrier for the “reverse” reaction would need to be decreased by ca. 6 kcal/mol on the oxygen covered surface. This value compares to that for the increased heat of adsorption on O-covered surfaces reported in the literature. In summary, the effect of surface oxygen on the kinetics of the interconversion of ethylene and oxametallacycles appears to be greater than on the reactions of oxametallacycles to oxygen-containing products, including ethylene oxide. The information captured in Figure 1 represents the next level of detail that needs to be represented in the reaction network illustrated above.

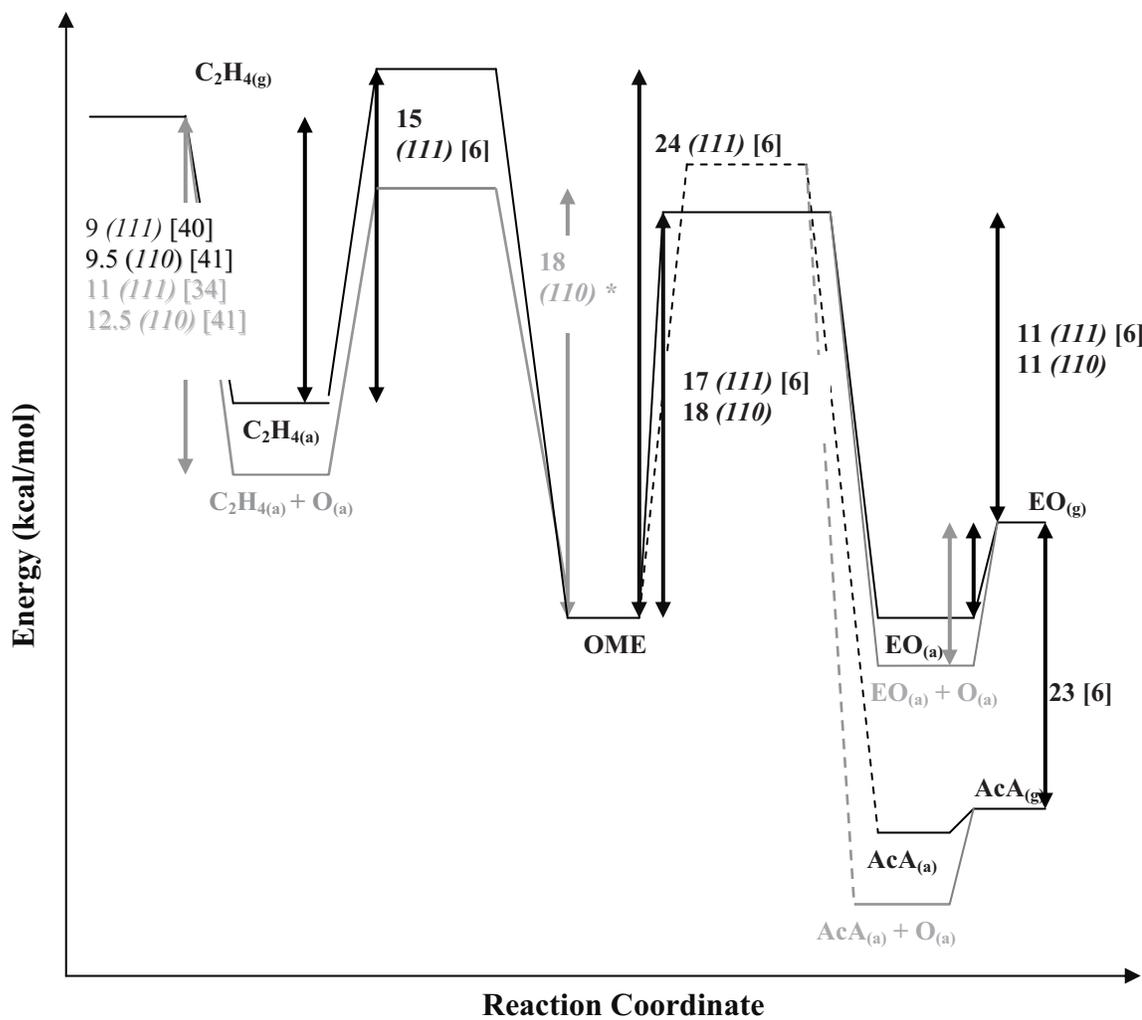


Figure 1. Reaction coordinate of ethylene oxide-derived oxametallacycles on the clean (black lines) and oxygen-covered (gray lines) Ag surfaces.

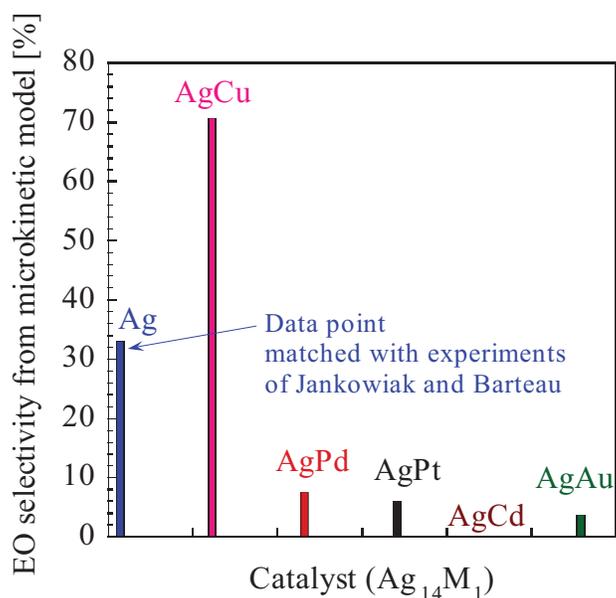
For **computational design of bimetallic catalysts**, we have utilized both periodic slab and finite cluster DFT calculations. DACAPO and Amsterdam Density Functional (ADF) packages were used for the respective methods. Given the optimized configurations of adsorbed reactants and products, the Nudged Elastic Band (NEB) method in DACAPO was employed to find the transition state and the corresponding activation energy barrier. These calculations were significantly CPU intensive (CPU ~ 15000 hours) and all such calculations were been performed on MPP2 at PNNL.

We have explored the predicted differences in activation energies for EO and acetaldehyde formation for bimetallics including silver and its neighbors in the Periodic Table (e.g., Cu, Pd, Pt, Cd, Au, Rh, Ir, Ni, Zn, and Os). In this study, we replaced one Ag atom bonded to the oxygen of the oxametallacycle with an M atom to generate a bimetallic  $\text{Ag}_{14}\text{M}_1$  cluster. Single point energy calculations were carried out using ADF for the reactant, 10 images along the reaction coordinate, and the product, for each of the oxametallacycle reaction channels.

$\text{Ag}_{14}\text{Cu}_1$ ,  $\text{Ag}_{14}\text{Pd}_1$ , and  $\text{Ag}_{14}\text{Pt}_1$  were predicted to be more selective than pure Ag, whereas all other bimetallic catalysts were more prone to form acetaldehyde. Au is known to decrease the selectivity and our DFT predicted results indicated the same. From the previous experimental studies in our group, Cu-Ag bimetallic catalysts were found to be more selective than pure Ag and this computational study also confirmed that. Clearly, this simple idea of assuming same transition state structures on different low loading bimetallic catalysts provides trends consistent with available experimental observations and simultaneously results in tremendous CPU savings.

Even though DFT results are useful in obtaining trends in EO selectivity by calculating activation energies, there are additional factors controlling the selectivity. For example, the pre-exponential factors and the magnitude of activation energies can also influence the selectivity. We therefore incorporated the results above into a more complete microkinetic model represented by the network above in order to predict the effect of different bimetallic combinations on both activity and selectivity.

The results are shown in Figure 2. AgCu shows higher EO selectivity than that on pure Ag, consistent with the DFT calculations. Similarly, AgCd and AgAu show lower EO selectivity than that on pure Ag, also consistent with the DFT calculations. However, AgPd and AgPt did not turn out to be better catalysts than pure Ag. It is observed that apart from the differences in activation energies, pre-exponential factors, and magnitudes of activation energies, stability of the OME is another factor controlling the selectivity. OME stability on  $\text{Ag}_{14}\text{Pd}_1$  and  $\text{Ag}_{14}\text{Pt}_1$  is much higher than that on other catalysts, which results in almost zero activation energy for OME formation from adsorbed EO. In comparison, the activation energy for OME formation from adsorbed acetaldehyde is more than acetaldehyde desorption, so the EO selectivity decreases significantly on these two catalysts. Overall, AgCu is the only bimetallic catalyst showing higher EO selectivity than pure Ag, based on microkinetic analysis.



**Figure 2:** Predictions of EO selectivity on different bimetallic  $Ag_{14}M_1$  catalysts using microkinetic modeling. Pre-exponential factors are adjusted to correctly capture the experimental EO selectivity on pure Ag.

In summary, the combination of DFT calculations for the selectivity-controlling steps with microkinetic models for the complete reaction have successfully identified a new bimetallic catalyst for ethylene epoxidation, while helping to eliminate “false positives” from our initial computational screening.

## SUMMARY

The work carried out under this grant has significantly advanced the field of catalyst design from first principles. The combination of computational tools, surface science, and catalytic reactor experiments in a single laboratory has few other examples. We have successfully predicted and validated new bimetallic catalyst for ethylene epoxidation. In so doing, we have established one of the first examples of successful catalyst design from first principles to achieve improved reaction *selectivity*. We are confident that others will follow this path!

*Publications resulting from FG02-84ER13290, 2006-2009*

SOLE FUNDING

1. M. A. Barteau, "Surface Science and the Advancement of Direct Olefin Epoxidation," *Surface Science*, **600**, 5021 (2006).
2. S. Linic and M. A. Barteau, "Heterogeneous Catalysis of Alkene Epoxidation," Chapter 14.11.6 in the *Handbook of Heterogeneous Catalysis*, 2<sup>nd</sup> edition, G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp (eds.), Wiley-VCH, (2008) pp. 3448-3464.
3. A. Lukaski, M. C. N. Enever, and M. A. Barteau, "Structure and Reaction of Oxametallacycles Derived from Styrene Oxide on Ag(110)," *Surface Science*, **601**, 3372 (2007).
4. A. C. Lukaski and M. A. Barteau, "Investigation of Ethylene Oxide on Clean and Oxygen-Covered Ag(110) Surfaces," *Catalysis Letters*, **128**, 9 (2009).

JOINT FUNDING (with FG02-03ER15468)

5. A. B. Mhadeshwar and M. A. Barteau, "Computational Strategies for Identification of Bimetallic Ethylene Epoxidation Catalysts," in *Mechanism in Homogeneous and Heterogeneous Epoxidation Catalysis*, S. T. Oyama (ed.), Elsevier (2008) p 265.
6. J. C. Dellamorte, J. Lauterbach and M. A. Barteau, "Rhenium Promotion of Ag and Cu-Ag Bimetallic Catalysts for Ethylene Epoxidation," *Catalysis Today*, **120**, 182 (2007).
7. J. C. Dellamorte, M. A. Barteau and J. Lauterbach, "Opportunities for Catalyst Discovery and Development: Integrating Surface Science and Theory with High Throughput Methods," *Surface Science*, **603**, 1770 (2009).
8. J. C. Dellamorte, J. Lauterbach and M. A. Barteau, "Effect of Preparation Conditions on Ag Catalysts for Ethylene Epoxidation," *Topics in Catalysis* (in press).
9. J. C. Dellamorte, J. Lauterbach and M. A. Barteau, "Promoter-induced morphological changes of Ag Catalysts for Ethylene Epoxidation," *Industrial and Engineering Chemistry Research*, **48**, 5943 (2009).

*Invited Lectures*

Distinguished Research Lecture, Department of Chemical Engineering, Carnegie Mellon University (February 2006).  
Department of Chemical Engineering, Ohio State University (May 2006).  
Department of Chemical and Biomolecular Engineering, University of Illinois (September 2006)  
Department of Chemical Engineering and Materials Science, University of Minnesota (November 2006).  
American Vacuum Society (November 2006)  
New Zealand Institute of Chemistry (December 2006)

School of Chemical Engineering, Purdue University (February 2007)  
Department of Chemical Engineering, University of Houston (March 2007)  
Donald L. Katz Lectures, Department of Chemical Engineering, University of Michigan (April 2007)  
2007 Catalytic Advances Program, The Catalyst Group Resources, Houston, TX (June 2007)  
Sasol Technology Ltd., Sasolburg, South Africa (July 2007)  
Symposium on Mechanisms in Homogeneous and Heterogeneous Catalytic Epoxidation, ACS National Meeting (August 2007)  
Department of Chemical Engineering, Lehigh University (September 2007)  
Department of Chemical Engineering, University of Connecticut (December 2007)  
Department of Chemical Engineering, Princeton University (January 2008)  
Department of Chemical Engineering, Case Western Reserve University (April 2008)  
Keynote Lecture, 14<sup>th</sup> International Congress on Catalysis, Seoul, South Korea (July 2008)  
A Century of Surface Science and Catalysis, AIChE Centennial Meeting, Philadelphia, PA (November 2008)  
D. B. Robinson Distinguished Speaker, Department of Chemical and Materials Engineering, University of Alberta (February 2009, scheduled)  
Somorjai Award Symposium, ACS National Meeting (March 2009)  
Murphree Award Symposium, ACS National Meeting (March 2009)  
Parravano Award Lecture, Michigan Catalysis Society (May 2009)

### *Recognition*

2009	Guiseppe Parravano Award, Michigan Catalysis Society
2008	Named as one of the “One Hundred Engineers of the Modern Era” by the American Institute of Chemical Engineers
2006	National Academy of Engineering

Professor Barteau was appointed Senior Vice Provost for Research and Strategic Initiatives at the University of Delaware, effective July 1, 2008.