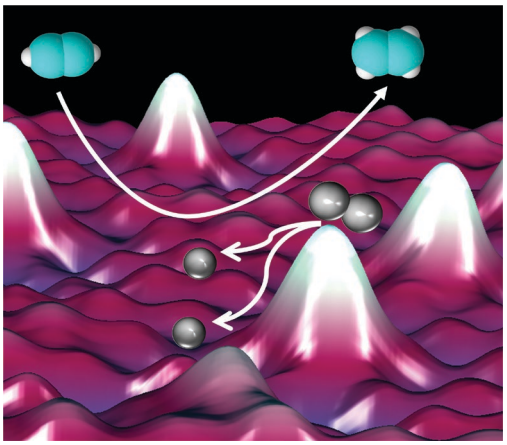
Single-Atom Alloy Catalysts: Born in a Vacuum, Tested in Reactors, and Understood In Silico

E. Charles H. Sykes

Tufts University, Department of Chemistry, 62 Talbot Ave, Medford, MA 02155, USA
charles.sykes@tufts.edu

In this talk I will discuss a new class of heterogenous catalysts called *Single-Atom Alloys* in which precious, reactive metals are utilized at the ultimate limit of efficiency.[1-6] These catalysts were discovered by combining atomic-scale scanning probes with more traditional approaches to study surface-catalyzed chemical reactions. This research provided links between atomic-scale surface structure and reactivity which are key to understanding and ultimately controlling important catalytic processes. In collaboration with Maria Flytzani-Stephanopoulos these concepts derived from our surface science and theoretical calculations have been used to design *Single-Atom Alloy* nanoparticle catalysts that are shown to perform industrially relevant reactions at realistic reaction conditions. For example, alloying elements like platinum and palladium with cheaper, less reactive host metals like copper enables 1) dramatic cost savings in catalyst manufacture, 2) more selective hydrogenation and dehydrogenation reactions, 3) reduced susceptibility to CO poisoning, and 4) higher resistance to deactivation by coking. I go on to describe very recent theory work by collaborators Stamatakis (UCL) and Michaelides (Cambridge University) that predicts reactivity trends for a wide range of *Single-Atom Alloy* combinations for important reaction steps like H-H, C-H, N-H, O-H, and CO_2 activation. Overall, I hope to highlight that this combined surface science, theoretical, and catalyst synthesis and testing approach provides a new and somewhat general method for the a priori design of new heterogeneous catalysts.



Scanning tunneling microscope (STM) image showing atomically-dispersed palladium atoms in a copper surface. The palladium atoms activate hydrogen enabling the industrially important acetylene-ethylene conversion with 100% selectivity.

References:
[1] Kyriakou et al. Science **335**, 1209 (2012).
[2] Marcinkowski et al. Nature Materials **12**, 523 (2013).
[3] Lucci et al. Nature Communications **6**, 8550 (2015).
[4] Liu et al. JACS **138**, 6396 (2016).
[5] Marcinkowski et al. Nature Chemistry **10**, 325 (2018).
[6] Hannagan et al. Science **372**, 1444 (2021).