ATOM-EFFICIENT NANOCATALYSTS FOR POINT-OF-NEED APPLICATIONS: POTABLE WATER TREATMENT AND FLARE GAS REDUCTION

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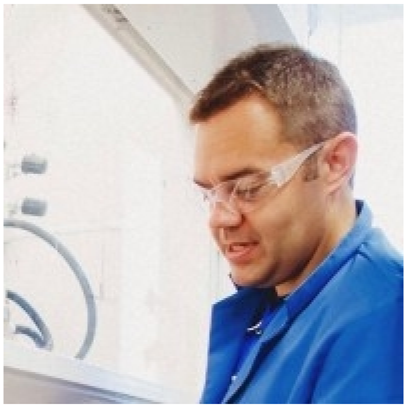

Abstract: The majority of large-scale industrial catalytic processes conducted at refinery sites rely on precious metal heterogeneous catalysts. This practice remains both economically and environmentally viable from the perspective of the catalyst materials, because precious metal recovery and recycling from spent catalysts is nearly 100% efficient. Furthermore, major chemical companies rent precious metals from merchant banks and other sources, so there is a limited drive to convert to the use of more atom-efficient catalysts, or those based on more ‘earth abundant’ metals. In stark contrast, however, catalytic reactions that are required to be conducted on smaller scales and in remote locations do require the discovery of new, alternative catalyst materials, since the economics of small-quantity catalyst recovery from multiple locations is problematic. The dilution of precious metals (e.g., Ru, Re, Rh, Ir, Pd, Pt) with less scarce and catalytically less relevant coinage metals (i.e., Cu, Ag) is one route to preparing more atom-efficient catalysts. However, in many cases, combinations of such metals result in classically immiscible (or metastable) alloys, which tend to segregate, either spontaneously, or under catalytic conditions. The formation of nanoscale metal alloys is one way to ‘kinetically trap’ such metastable structures, by taking advantage of confinement effects at the nanoscale. In our work, we have shown how microwave-assisted heating can be used to prepare a broad range of binary and ternary metal alloy nanoparticles, which are stable under catalytic conditions, and which can exhibit reactivity enhancement based on synergistic alloying effects. We use experiment and DFT to understand reactivity of such novel catalysts under a range of conditions. Of direct relevance to the current meeting, in recent years, we have focused in particular on using metal alloy nanoparticles for two challenges that directly relate to point-of-need catalysis. In the first case, we have studied the use of our alloy catalysts in waste water remediation for return to municipal dirking water, via removal of toxic species including nitrate, nitrite and bromate by hydrogenation catalysis. In the second case, we are presently exploring the use of a sub-set of specific metal alloy catalysts for the controlled activation of natural gas (i.e., CH4) to CH3 and H,to subsequently form liquid C1 products (e.g., CH3OH, CH3CO2H). At present, natural gas generated at remote oil recovery sites is combusted, releasing CO2 into the atmosphere, because capture, liquification, and/or transportation of CH4 is

not economically viable on a small scale. In contrast, if modular catalytic reactors could be deployed to generate stable liquid fuels on-site, value-added byproducts could be generated, whilst concomitantly negating direct CO2 generation.

Bio: Dr. Simon Humphrey was born in Wisbech, England in 1979. As an undergraduate he attended The University of East Anglia, Norwich (1998−2002) and The University of California at Santa Barbara (2000−2001) and obtained a Master of Chemistry degree (MChem, Class I). He then moved to The University of Cambridge (2002−2005) as a graduate student at St John's College and obtained his Ph.D. studies under the supervision of Paul T. Wood, in the field of magnetic and porous coordination polymer synthesis. He then worked under the co-supervision of T. Don Tilley and Gabor A. Somorjai as a US Department of Energy Postdoctoral Research Associate at the Lawrence Berkeley National Laboratory (2005−2007), in the field of nanoparticle catalysis. In 2006, he undertook a Fellowship at St John's College, Cambridge, before joining the Faculty at the University of Texas at Austin as an Assistant Professor in 2009. He is currently Professor and holds the W. H. Wade Professorship in Chemistry. He is an editor for Coordination Chemistry Reviews, and serves as CTO for the startup company Lantha, Inc., based in Austin, which uses MOFs as chemical sensors.