**Title**

Understanding implications of catalyst electronic structure: Nitrate reduction as a model case

**Abstract**

Ammonia produced by the Haber-Bosch process fixes nitrogen by sourcing hydrogen from methane steam reforming—today’s most carbon intensive industrial process. Alternatively, ammonia can be produced electrochemically from industrial waste nitrogen sources (e.g. nitrogen oxides including nitrate), sourcing protons from water and electrons as reducing agents. However, reduction of such oxidized nitrogen species involves complex reaction mechanisms where the stability of critical reaction intermediates (e.g. nitric oxide) dictates selectivity towards ammonia as a final product. Here we evaluate the role of transition metal bulk resting electronic structure (*d*-band center energy and work function) on nitrate reduction reaction Faradaic efficiency and selectivity to ammonia. We frame our discussion of these results within theoretical and empirical literature on hydrogen evolution and nitric oxide adsorption, finding work function dictates total nitrate reduction Faradaic efficiency while *d*-band center energy describes selectivity towards ammonium. We further support these observations with synchrotron-based ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) to explore the adsorption affinity, and ability of a surface to dissociate, nitric oxide for a series of transition metals (Fe, Co, Ni, Cu).

**Bio**

Quinn Carvalho is a fifth year Ph.D. student in the Stoerzinger research group at Oregon State University. His research focuses on developing relationships between catalytic performance and material physicochemical parameters for the cyclic and renewable conversion of waste nitrate into value added chemical commodities such as ammonia. As part of his PhD, he has been recognized as a DOE SCGSR fellow, spending one year at the Advanced Light Source, and is the recipient of several scientific communication awards from regional and national conferences.