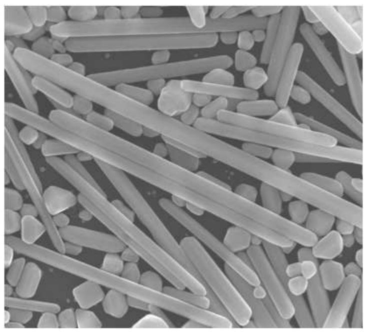
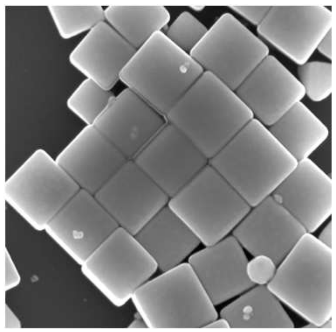
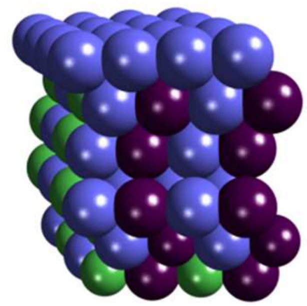
From first principles studies to novel electro-catalysts for oxygen reduction reaction: design, synthesis and testing.

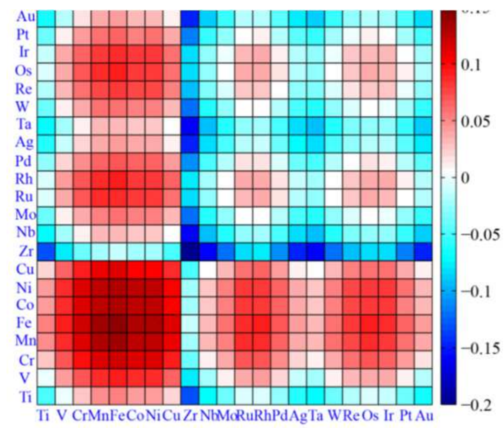
Suljo Linic, Department of Chemical Engineering, University of Michigan, Ann Arbor, Mi

The project focuses on finding alternatives to Pt electro-catalysts in electrochemical oxygen reduction reaction (ORR). The focus is on designing, synthesizing, and testing two families of materials. The design of electro-catalysts is guided by first principles quantum chemical calculations.









One family of materials are Ag nanoparticles of exotic shapes (including nanowires and nanocubes). These materials are terminated with more active Ag surfaces (manly the 100 surface) than spherical Ag particles, and it principle these materials should be more active in ORR

Another family of materials are alloy containing Ag. The design of optimal alloys is guided by quantum chemical calculations, which based on molecular models for this reaction, can be used to suggest optimal composition for the active site.