***Computational study of water oxidation at cobalt oxide surfaces.* (Mentor: Hrant P. Hratchian)** A key question in the development of solar energy based technologies is the conversion of energy from photons into another form for storage. A favored design approach is the conversion of this energy into the internal chemical energy of H_2. Such an approach would produce a high energy density fuel that can be generated from a carbon-free and abundant feed stock, namely water. A critical and remaining chemical challenge is the development of an economical, robust, and efficient water oxidation catalyst. One recent exciting breakthrough has been the introduction of cobalt-based thin film catalysts. Developed by Nocera and others, these catalysts exhibit a number of highly desirable design highlights. Among these features are that they employ an earth-abundant metal, operate with neutral water at room temperature, and appear to be self-healing. Indeed, a recent report shows how these catalysts can be incorporated in constructing an *artificial leaf* device.

Experimental results indirectly suggest that the catalyst thin films are comprised of edge-sharing CoO_6 octahedral structural units. This system is well-suited for computational study using the cluster model approach used in investigations of semiconductor and insulator surface chemistry. Employing such a model, students will examine aspects of the catalyst preparation and structure. Some of these processes include: (1) the initial deposition step on substrates such as WO_3 and ZnO; (2) growth of the film layers from Co^{2+}, phosphate, and water; and (3) potential for alkali metal inclusion in the cubane structure similar to the presence of Ca^{2+} in the photosystem II oxygen evolving complex and colbaltates. Importantly, this project can be easily catered to the specific background and interests of the involved student(s).