THE PARTNERSHIP FOR INTERNATIONAL RESEARCH AND EDUCATION AT THE UNIVERSITY OF CALIFORNIA
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SEMINAR ANNOUNCEMENT

Design of targeted nanostructures for efficient and environmentally friendly catalysis and photo-catalysis

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ABSTRACT

Materials for almost all commercial heterogeneous catalytic, electro-catalytic, and photo-catalytic processes have been designed through trial and error experimental approaches. This approach to discovery has led to many commercial processes which are environmentally unfriendly, have high overall activation barriers (rendering them less energy efficient), and are limited by low selectivity. In our research group we have been developing strategies for the 'rational', bottom-up design of solid materials for energy-efficient and environmentally friendly chemical transformations. We are motivated by a realization that recent scientific advancements, mainly in the area of molecular science, are bringing a revolutionary transformation to the fields of heterogeneous catalysts, electro-catalysis, and photo-catalysis. The landscape-changing advances driving the transformation are:

(i) Development of powerful spectroscopy and microscopy techniques, allowing us to study chemical transformations on catalytic particles with high spatial and temporal resolutions and at relevant conditions,
(ii) Development of quantum computational methodologies (for example, Density Functional Theory (DFT)), which can be utilized to study chemical transformations at the elementary step level with reasonable accuracy and efficiency. These tools are allowing us for the first time to make reasonable quantitative predictions about the outcome of elementary chemical surface reactions,
(iii) Development of novel synthetic chemistry approaches designed to synthesize targeted nano-structured materials with almost atomic precision and with a high degree of uniformity.

I will show a few examples where we used the above-mentioned advancements to design, synthesize, and test targeted nano-structures for energy-efficient and environmentally friendly catalytic and photo-catalytic chemical transformations. I will discuss partial oxidation of olefins to form epoxides over well-defined silver nano-particles of targeted shapes (spheres, wires, and cubes). I will show how we used DFT quantum chemical calculations to identify optimal catalytic sites (these are intimately related to the shape of Ag particles). Furthermore, I will illustrate our approach to the controlled synthesis of these catalytic sites. In the second example, I will show that composite photo-catalysts combing shaped metallic nano-particles of noble metals (Au or Ag) and semiconductor nanostructures (for example TiO_2) exhibit significantly improved photo-chemical activity compared to conventional photo-catalytic materials. The critical feature of these composite photo-catalyst is that they couple excellent optical absorption properties of shaped metallic nanostructures (Au or Ag), manifested in the formation of surface plasmons in response to a photon flux, and photo-catalytic potential of semiconductors, therefore enabling more efficient conversion of solar flux into electron/hole pairs. The advantage of the composite photo-catalysts will be discussed in the context of photo-catalytic conversion of solar energy into chemical energy of solar fuels by photo-electro-chemical splitting of water to form H_2 and O_2. Finally, I will illustrate how plasmonic metallic nanostructures can concurrently use low intensity visible light and thermal stimuli to drive catalytic reactions at lower temperature than their conventional counterparts that use only thermal stimuli. The results open avenues towards the design of more energy efficient and robust catalytic processes.

Refreshments will be served before the seminar

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