Physical Chemistry Seminar

Tuesday, February 23, 2010 | **11:00 a.m.** | **Room 1315 Chemistry Building**

Locally Modified Oxide Catalysts

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Oxides are used as catalysts for the oxidation and the oxidative dehydrogenation of various organic compounds. We use density functional theory and experiments to determine whether we can improve the catalytic activity of an oxide by making local modifications of their surface. We have considered so far three kinds of modifications: a) some of the cations in the oxide are replaced with a different kind of cation (cation doping), b) some of the anions in the oxide are replaced with a different anion (anion doping) and c) isolated, single-cation oxide clusters are supported on the surface of another oxide. We have shown that cation doping can modify the catalytic activity of the host oxide through three mechanisms: 1) the presence of the dopant weakens the bond of the nearby oxygen atoms to the surface and makes the system a stronger oxidant; 2) the valence of the dopant is not satisfied and it adsorbs oxygen from the gas phase activating it to make it a better oxidant; 3) an appropriate choice of the dopant and of the host oxide facilitates dissociative adsorption of gas-phase molecules. We have used doped oxides to study CO oxidation, partial oxidation of the methane and dry reforming of methane. We have also studied methanol oxidation by VO_3, CrO_3 and MoO_3 clusters adsorbed on titania. We have calculated the likely structure of these clusters and the mechanism of methanol conversion to formaldehyde. I will also report preliminary experiments in which we deposit mass selected VO and VO_2 clusters on TiO_2(110).

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:15 p.m. in Room 8305f