TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

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IAP-SEMINAR

EINLADUNG

Termin: **Mittwoch, 27.6.2012 um 16:00 Uhr**
Ort: **Technische Universität Wien,**
Institut für Angewandte Physik,
Seminarraum 134, Turm B (gelbe Leitfarbe), 5. OG
1040 Wien, Wiedner Hauptstraße 8-10

Vortragende: **Prof. Annabella Selloni**
Department of Chemistry, Princeton University, Princeton, NJ 08544

Thema: **Materials-related aspects of photocatalysis: insights from quantum simulations**

Kurzfassung

Environmental and energy-related issues have prompted considerable interest in photocatalysis over the last decade. In the search for new materials and processes capable of improving existing technologies, theory and computational modeling have proven useful tools which can contribute microscopic insights sometimes difficult to obtain by experiment. In this talk I will discuss applications of ab initio electronic structure calculations and molecular dynamics simulations to understand materials properties and reaction mechanisms relevant to photocalysis and energy applications. Examples will focus on bulk and surface properties of TiO_2, a widely used photocatalyst capable of splitting water in O_2 + H_2, and the spinel cobalt oxide Co_3O_4 a magnetic semiconductor which has recently attracted attention as a promising catalyst for low-temperature CO oxidation, water splitting, and the oxygen reduction reaction.

Alle interessierten Kolleginnen und Kollegen sind zu diesem Seminar
(45 min mit anschließender gemeinsamer Diskussion) herzlich eingeladen.

U. Diebold e.h.
(Seminar-Chairperson)

H. Störi e.h.
(LVA-Leiter)