FOXSI
Functional Oxide Surfaces and Interfaces

EINLADUNG

zum Vortrag
von

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Materials-related aspects of photocatalysis: insights from quantum simulations

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Mittwoch, 27. Juni 2012, um 16:00

Technische Universität Wien, Institut für Angewandte Physik
Seminarraum 134A, Turm B (gelbe Leitfarbe), 5. OG
1040 Wien, Wiedner Hauptstraße 8-10

Abstract:

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.

FWF SFB F45 „Functional Oxide Surfaces and Interfaces (FOXSI)“
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