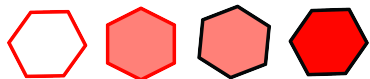


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ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

NCCR MARVEL Distinguished Lecture

Photocatalysis on TiO₂: insights from simulations

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Tuesday 16th May 2017, 16:15, Room MXF-1

Abstract: TiO₂-based photocatalysis for the degradation of pollutants and the splitting of water into H₂ and O₂ has been an important area of research for decades. In this talk I shall discuss recent applications of first principles electronic structure calculations and molecular dynamics simulations to understand materials properties and reaction mechanisms in TiO₂-based heterogeneous photocatalysis. Examples will focus on the structure and reactivity of anatase TiO₂ aqueous interfaces, the behavior of charge carriers at the interface, and the formation and structure of so-called black TiO₂, a promising functional material capable to absorb the whole spectrum of visible light.