UNIVERSITA' DEGLI STUDI DI PERUGIA
Dipartimento di Chimica, Biologia e Biotecnologie

AVVISO DI SEMINARIO

Lunedì 20 giugno ore 15.00

aula B, edificio A, via Elce di Sotto 8

Prof. Annabella Selloni

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"Using numerical simulations to understand materials and processes in photo- and electro-catalysis"

Environmental and energy-related concerns have prompted considerable interest in photo- and electro-catalysis over the last years. In the search for new materials and processes capable of improving existing technologies, theoretical and computational modeling can provide microscopic insights sometimes difficult to obtain by experiment. In this talk I will discuss applications of first principles electronic structure and molecular dynamics simulations to understand materials properties and reaction mechanisms in photo- and electro-catalysis. Examples will include studies of the interface between water and titanium dioxide (TiO_2), a widely used photocatalyst capable of splitting water in O_2 + H_2, and H_2 production by a bio-inspired catalyst-electrode complex in water.

Tutti gli interessati sono invitati a partecipare

Dott. Francesca Nunzi

Francesca Nunzi