Title:
Characterization of photoelectrodes through computer simulations

Abstract:
In this talk, I will show how computer simulations based on first principles can provide insight into crucial processes for energy conversion taking place at the photoelectrode and at the interface between photoelectrode and electrolyte in photoelectrochemical cells. Relations between atomic structure of the system and photoabsorption, charge transfer, and chemical reactivity are investigated, and lead to a deeper understanding of the functional behaviour of the materials. These results help the interpretation of electrochemical measurements, and may guide the development of better photoelectrodes.

Short bio:
Nicola Seriani is **staff scientist** at the **Abdus Salam International Centre for Theoretical Physics, Trieste, Italy**. His research is dedicated to the investigation of materials, mostly transition metals and their oxides, of relevance for heterogenous catalysis, energy conversion and storage, by means of atomistic computer simulations based on first principles. In the last years, he has focused on oxygen evolution and reduction reactions in the context of hydrogen production from water and of metal-air batteries. He holds a degree in physics from the University of Trieste and a Ph.D. in materials engineering from the Dresden University of Technology; he worked several years at the University of Vienna. He is chairman of the executive committee of the African School on Electronic Structure Methods and Applications.