The Abdus Salam
International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

WORKSHOP ON NEW MATERIALS FOR RENEWABLE ENERGY
17 - 21 October 2011, ICTP, Trieste

FIRST-PRINCIPLES MODELING OF ELECTROCHEMICAL REACTIONS FOR SOLAR-TO-FUEL ENERGY STORAGE

Simone PICCININ
S.I.S.S.A. Scuola Internazionale Superiore di Studi Avanzati
Trieste, Italy

ABSTRACT 1:

Through photosynthesis, plants are able to use sunlight to promote electrochemical reactions that convert water and carbon-dioxide into sugars. An analogous artificial process could be exploited to convert and store solar energy in the form of fuels such as hydrogen or methanol [1]. Complex electrochemical reactions take place at both electrodes of such a device, and suitable catalysts are needed to handle the stringent thermodynamic and kinetic requirements. Modeling these processes from first-principles is a formidable challenge and in this talk I will briefly review some of the recent progress made in the field. In particular I will describe some techniques [2,3] to compute reaction free energies of electrochemical reactions and how they have been applied to the study of water oxidation and oxygen reduction reactions.

[1] V. Balzani, A. Credi, M. Ventura, ChemSusChem 1, 26 (2008)
[2] J. Norskov et al., J. Phys. Chem. B 108, 17886 (2004)
[3] X. Yang and M. Baik, J. Am. Chem. Soc. 126, 13222 (2004)