WISE
WATERLOO INSTITUTE
FOR SUSTAINABLE ENERGY

LECTURE SERIES

Presented by the Waterloo Institute for Sustainable Energy

Wednesday, June 6, 2012
10:30 – 11:30A
DC 1304

Computational Chemistry and the Design of Dye Sensitized Solar Cells

Dr. Carlo Adamo
Chair of Theoretical Chemistry
Senior Member of Institute Universitaire de France (IUF)

A step-by-step theoretical protocol based on DFT at both molecular and periodic levels is proposed for assisting the design of DSSC devices. This computational tool is tested and discussed for ZnO and TiO2 based DSSCs. First, the ability of DFT for the prediction of the UV-Vis spectrum of isolated dyes will be discussed. Then the electronic structure of the dye adsorbed on the oxide semiconductor's surface will be considered, also including solvent and electrolyte additives effects.

Our stepwise protocol was successfully validated by the consistency with experiments. This procedure should be useful not only as a complement to experimental approaches but also for lightening them as regards time and resource consumption.

Biography

Carlo Adamo completed his Masters and Ph.D. degrees in Chemistry and Theoretical Chemistry at the University of Naples, Italy, in 1990 and 1995, respectively. He is currently the Chair of Theoretical Chemistry and a Senior Member of the Institute Universitaire de France (IUF). His main research interests concern the development of DFT approaches and their applications in the field of energy production. Dr. Adamo is the author of 235 papers in international peer-review journals. He has been a co-author of the computer codes Gaussian since 1998. He is a Member of the Advisory Board of Physical Chemistry Chemical Physics.