

Devis Di Tommaso



Marie-Curie Research Fellow at
Department of Chemistry and Material Simulation
Laboratory
University College London

February 2006 – February 2007 :
Post-Doctoral / Research Associate at
Davy Faraday Research Lab., The Royal Institution of
GB

March 2006 :
Ph.D. in Quantum Chemistry, University of Trieste
(Italy), Department of Chemistry

Bio

Scientific Interests and Research Activities:

General research field

Computer modelling of materials through density functional theory, ab initio and Car-Parrinello molecular dynamics methods.

Current research topics:

- Reactivity in aqueous solution.
- Homogeneous nucleation of calcium carbonate from aqueous solution.
- Oligomerisation process of phosphates species.

Recent and previous research topics:

- Computational study of organometallic catalysts for the asymmetric hydrogenation of ketones.
- Elucidation of the factors controlling enantioselectivity in ruthenium catalysts.
- Mechanism of asymmetric transfer hydrogenation reaction in aqueous solution.
- Density functional theory study of molecular photoionization processes using a locally developed density functional theory B-spline LCAO method.
- Computational study of circular dichroism in the angular distribution of photoelectrons emitted from chiral molecules.
- Investigation of branching ratios deviations from statistical behaviour in core photoionization.
- Development and numerical implementation of a theoretical methodology for the localization and characterization of "shape resonances".