CURRICULUM VITAE

E. D. Simandiras

Senior Researcher
Theoretical and Physical Chemistry Institute

+30-210-7273806
msim@eie.gr
ResearcherID F-8867-2012

My research interests lie in the field of Molecular Electronic Structure Theory and Computational Chemistry.
I was educated at the Leonteion Lykeion School of Nea Smyrni (class of '79) and then in Chemistry at the University of Athens (Ptyhio 1984). I then did my Ph. D. research work in the Department of Theoretical Chemistry at the University of Cambridge with Nick Handy. The title of my thesis is "Analytic Energy Derivatives" and was funded under the EEC "Stimulation Action" program. I obtained my Ph. D. degree in 1987.
After a short postdoctoral employment at the University of Cambridge I returned to Greece for my Military service (1988-90 at the Research and Development Office of the Greek Navy).
Since 1990 I am a researcher at the Theoretical and Physical Chemistry Institute of the NHRF, working on various aspects of ab initio Electronic Structure Theory applications. I have also been actively involved in the setup and management of all the computational systems of the Institute during this time.
A couple of selected publications representative of my old development days are:

- "On the high accuracy of MP2 optimised geometries and harmonic frequencies with large basis sets", E D Simandiras, R D Amos and N C Handy, Chem. Phys. Lett. 133, 324(1987).
- "On the necessity of f basis functions for bending frequencies", E D Simandiras, J E Rice, T J Lee, R D Amos, and N C Handy, J. Chem. Phys. 88, 3187 (1988).

The first one has been cited about 90 times and the second more than 170.

My recent projects involve the theoretical investigation of amorphous inorganic systems, and also theoretical studies of transition metal clusters with an interest on catalysis. Representative publications for the first subject are:

- "Theoretical study of glass systems using ab initio Molecular Electronic Structure Theory. 1. Lithium metaphosphate glass", E.D. Simandiras and D.G. Liakos, J. Phys. Chem. A 108, 3854 (2004).
- "Theoretical Study of Glass Systems using Molecular Electronic Structure Theory. 2. Structure and Spectroscopy of the B2O3 Glass", D. G. Liakos and E. D. Simandiras, J. Phys. Chem. A 112, 7881 (2008)

and for the second:

- "A theoretical study on the solvolytic reactivity of the [Re3(μ-Cl3)Cl9]n- clusters (n=3,4) using ab initio and density functional theory calculations", N. Psaroudakis, K. Mertis, D. G. Liakos and E. D. Simandiras, Chem. Phys. Lett. 369, 490 (2003).
- "Theoretical investigation of the stepwise hydrolysis of the [Re3(μ-Cl3)Cl9]3- Anion", D.G. Liakos, E.D. Simandiras, N. Psaroudakis and K. Mertis, Inorg. Chem., 46 (6), 2167 (2007).

The latter subject is actively pursued leading to very interesting results. See:

- "Theoretical prediction of new Kubas four centre H_2 complexes involving dimolybdate clusters", E. D. Simandiras and D. G. Liakos, Chem. Phys. Lett. **583**, 18 (2013)
- "Theoretical Elucidation of a Classic Reaction: Protonation of the Quadruple Bond of the Octachlorodimolybdate(II,II) $[Mo_2Cl_8]^{4-}$ Anion", E. D Simandiras, M. Tsakiroglou, N. Psaroudakis, D. G. Liakos, and K. Mertis, Inorg. Chem., **51**, 258 (2012)

Full publication list can be found at
<script src='http://labs.researcherid.com/mashlets?el=badgeCont957980&mashlet=badge&showTitle=false&className=a&rid=F-8867-2012'></script>