

## Ioannis S. K. Kerkines

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### EDUCATION

- Ph.D. in Physical Chemistry, National and Kapodistrian University of Athens, Athens, Greece (2003)
- M.Sc. in Physical Chemistry, National and Kapodistrian University of Athens, Athens, Greece (1999)
- B.Sc. in Chemistry, National and Kapodistrian University of Athens, Athens, Greece (1997)

### RESEARCH AND TEACHING APPOINTMENTS

11/2013- : Postdoctoral Researcher, TPCI/NHRF, Athens, Greece  
 10/2008-12/2011: Postdoctoral Researcher, TPCI/NHRF, Athens, Greece  
 09/2006-08/2008: Postdoctoral Researcher, Emory University, Atlanta, GA, USA  
 08/2004-08/2006: Postdoctoral Researcher, National and Kapodistrian University of Athens, Athens, Greece

### MAIN RESEARCH INTERESTS

- Computational photochemistry and dynamics of molecules in excited states with applications in atmospheric and photovoltaic systems
- Theoretical study of chemical reaction mechanisms involving environmentally interesting processes
- Accurate quantum calculations on small molecules. Theoretical study of transition metal compounds with applications in material science
- Theoretical prediction of hitherto unknown stable chemical compounds with applications in noble-gas, polynitrogen, and nuclear chemistry

## TEACHING ACTIVITIES

- Teaching Assistant in the University of Athens (Physical Chemistry III, IV) (09/1998 - 06/2000)
- Teaching Assistant in the University of Athens (Introduction to Computers) (09/1998 - 06/2001)

## HONORS AND AWARDS

- 1998 Association of Hellenes from Egypt ( $\Sigma$ AE) scholar
- 09/1998-06/2002 Hellenic State Scholarships Foundation (IKY) scholar
- 09/2000 Scholarship and participation at the European Summerschool in Quantum Chemistry (ESQC 00) organized by Prof. B. O. Roos et al. in Riolo Terme, Italy
- 04/2001-06/2001, 05/2002-07/2002 Marie Curie fellow at the Jaroslav Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic with Prof. Petr Carsky
- 03/2008 Atlanta Area Chemical Physics (AACP) Award, Atlanta, USA
- 09/2010 QSCP Promising Scientist Award of CMOA nominee, Cambridge, UK.

## CONFERENCES AND SCIENTIFIC VISITS

- Over 25 original research papers in international peer-reviewed journals
- Over 30 announcements in international scientific conferences including WATOC, ICQC, QSCP, AFOSR, and ACS meetings
- 11/2004 Scientific visit to Jaroslav Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic (Prof. Petr Carsky)
- 10/2005 Scientific visit to ISOLDE/CERN, Geneva, Switzerland (Dr. Ulli Koster)
- 01/2009 Scientific visit to Universitat Karlsruhe, in Karlsruhe, Germany (Prof. Wim Klopper)

## SELECTED RECENT PUBLICATIONS

1. "Short- and long-range binding of Be with Mg in the  $X^1\Sigma^+$  ground state and in the  $A^1\Pi$  excited state", I. S. K. Kerkines and C. A. Nicolaidis, [J. Chem. Phys. 137, 124309 \(2012\)](#).
2. "Fluorescence properties of organic dyes: Quantum chemical studies on the green/blue neutral and protonated DMA-DPH emitters in polymer matrices", I. S. K. Kerkines, I. D. Petsalakis, P. Argitis, and G. Theodorakopoulos, [Phys. Chem. Chem. Phys., 13, 21273-21281 \(2011\)](#).
3. □ "Theoretical study on the electronic structure and the absorption spectra of complexes of  $C_{60}$  and  $C_{59}N$  with  $\pi$ -extended derivatives of tetrathiafulvalene", I.

D. Petsalakis, D. Tzeli, I. S. K. Kerkines, and G. Theodorakopoulos, [Comput. Theor. Chem. 965, 168-175 \(2011\)](#).

4. □ "Excited state intramolecular proton transfer in hydroxy oxime-based chemical sensors", I. S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos, and J. Rebek, Jr., [J. Phys. Chem. A 115, 834-840 \(2011\)](#).
5. □ "Li atoms attached to helium nanodroplets", A. Hernando, R. Mayol, M. Pi, M. Barranco, I. S. K. Kerkines, and A. Mavridis, [Int. J. Quantum Chem., 111, 400-5 \(2011\)](#).
6. □ "Experimental and theoretical study of the reaction of POCl<sub>3</sub><sup>-</sup> with O<sub>2</sub>", I. S. K. Kerkines, K. Morokuma, N. Iordanova, and A. A. Viggiano, [J. Chem. Phys. 132, 044309-9 \(2010\)](#).