

DEMETER TZELI

Research Associate,
Theoretical and Physical Chemistry Institute,
National Hellenic Research Foundation,
48 Vassileos Constantinou Ave.,
Athens 11635, Greece
Tel.: +30 210 6503313
Email: dtzeli@eie.gr



EDUCATION

B.Sc. 1995, M.Sc. 1997, Ph.D. 2000, all at the Department of Chemistry, National and Kapodistrian University of Athens.

RESEARCH APPOINTMENTS

Research Associate at TPCI/NHRF since 9/2006; Research Associate at IAMPPNM/Demokritos since 3/2013; Research Associate at Laboratory of Physical Chemistry, Department of Chemistry, NKUA 12/2000-8/2006; HPC- Europa Transnational Access programme (Research Associate Visitor, Theoretical Chemistry, Materials Science Center, Rijksuniversiteit Groningen, the Netherlands (10-11/2004); AWU fellow, PNNL, Richland, U.S.A. (7-9/1998); Summer School, Cornell University, Ithaca, N.Y., 7/1998.

TEACHING APPOINTMENTS

Laboratory Instructor, Physical Chemistry, at the Chemistry Department, University of Athens, 9/1996 - 6/1998. Teaching-Seminars of pc usage at Chemistry Department, University of Athens 5-12/1999 and KORELplus, Athens 11/2001-9/2002.

MAIN RESEARCH INTERESTS

Accurate *ab initio* calculations via MRCI and CCSD(T) methods on small molecules. Calculations of excited molecular states and their potential energy curves or surfaces, prediction of the spectra, calculation of the relativistic effects, etc.; i.e., diatomic and triatomic molecules including transition metals. Study of van der Waals systems, interactions of water with "hydrophobic" organic molecules via MP and CC methods. Study of large systems such as solid state and interactions of small molecules with surfaces mostly via DFT methods. Theoretical studies on supramolecular systems, fullerene crown ethers and complexes of porphyrins. Theoretical study of organic reactions. DFT calculations on magnetic materials, study of core/shell magnetic nanoparticles.

EXTERNAL FUNDING PROJECTS

COMANA "ARISTEIA" (27/3/2013 -); NATO Science For Peace And Security Programme (7/2009 - 7/2011); NANOHOST project, FP7 (5/2008-12/2011); Greek-Slovakian collaboration (9/2006-4/2008); HPC- Europa Transnational Access programme (10-11/2004); Pythagoras, EPEAEK II (7/2004-8/2006); SSATES, EPEAEK (5/1999-12/1999); AWU program (7-9/1998).

CONFERENCES AND INVITED TALKS

Participation in 17 international conferences (2 invited talks). Have given 5 invited talks at Universities.

HONORS AND AWARDS

Greek Award 2009 L'OREAL-UNESCO for the Women in Science; Fellowship of Academy of Athens (9/2002-6/2000); Associated Western Universities (AWU), USA, Laboratory Graduate Fellowship (7-9/1998); National Scholarship Foundation of Greece (11/1996-4/2000), National Scholarship Foundation of Greece (for academic achievement, 1991-1995); Scholarship of Women Association of Trikala (for achieving the highest score at the entrance examinations for the Chemistry Department, 1991-1992).

PROFESSIONAL AFFILIATIONS & ACTIVITIES

Editorial Board Member at *E-Journal of Chemistry*; Reviewer for scientific research proposals (Romanian National Research Council); Reviewer for scientific research journals in the fields of chemistry and materials science; Member of the Organizing Committee in 3 International Conferences; Member of the Association of Greek Chemists.

PUBLICATIONS

46 publications in refereed international scientific journals with 360 citations to the published work, h-index=11.

Full list of publications

Selected Publications

- "Electronic structure and bonding of the 3d-transition metal borides, MB, M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu through all electron *ab initio* calculations." D. Tzeli and A. Mavridis, *J. Chem. Phys.* 128, 034309(1-14) (2008).
- "The electron affinity of the gallium nitride (GaN) and digallium nitride (GaNGa). The importance of the basis set superposition error in strongly bound systems." D. Tzeli and A. A. Tsekouras, *J. Chem. Phys.* 128, 144103(1-7) (2008).
- "Theoretical study of adsorption of group IIIA nitrides on Si(111)." D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos *J. Phys. Chem. C* 113, 5563-5567 (2009).
- "Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a n-extended TTF derivative." D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *Phys. Chem. Chem. Phys.* 13, 11965 (2011).
- "Computational Insight into the Electronic Structure and Absorption Spectra of Lithium Complexes of N-confused Tetraphenylporphyrin." D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *J. Phys. Chem. A* 115, 11749 (2011).
- "Theoretical study of hydrogen bonding in homodimers and heterodimers of amide, boronic acid and carboxylic acid, free and in encapsulation complexes." D. Tzeli, G. Theodorakopoulos, I. D. Petsalakis, D. Ajami and J. Rebek, Jr *J. Am. Chem. Soc.* 133, 16977 (2011).
- "Conformations and fluorescence of encapsulated stilbene." D. Tzeli, G. Theodorakopoulos, I. D. Petsalakis, D. Ajami and J. Rebek, Jr *J. Am. Chem. Soc.* 134, 4346 (2012).