

## Giannoula Theodorakopoulos

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### EDUCATION

Ph.D in Physical Chemistry, Chemistry Department, University of Toronto, Toronto, Canada (1978)  
M.Sc. in Physical Chemistry, Chemistry Department, University of Toronto, Toronto, Canada (1974)  
B.Sc in Chemistry, Chemistry Department, University of Toronto, Toronto, Canada (1973)

### RESEARCH APPOINTMENTS & SABBATICALS

4/1998 - present	Director of Research, TPCI, NHRF, Athens, Greece.
1/1990-3/1998:	Senior Researcher, TPCI, NHRF, Athens, Greece.
5/1984-12/1989:	Research Assistant, TPCI, NHRF, Athens, Greece.
5/1978-4/1984:	Scientific collaborator, TPCI, NHRF, Athens, Greece.
1/2014-7/2014	Visiting position, Department of Chemistry, North Carolina State University (sabbatical leave)
9/2013–12/ 2013	Visiting position, The Fritz Haber Institute, The Hebrew University (sabbatical leave)
8/2002-7/2003	Visiting position, Chemistry Department, University of Toronto, Toronto, Canada (sabbatical leave)
8/1993-7/1995	Visiting position, Theoretical Chemistry Department, Oxford University, Oxford, U.K. (sabbatical leave)
8/1987-7/1988	Visiting position at the Chemistry Department, Carleton University, Ottawa, Canada. (sabbatical leave)

- 1979-1983 Long (2-5 months) visits to Physical Chemistry Institute, Bonn University, Bonn, Germany.
- 1983-2005 Long visits to Theoretical Chemistry Department, University of Wuppertal, Wuppertal, Germany.

### **MAIN RESEARCH INTERESTS**

Theoretical studies on fluorescent chemical sensors for dicarboxylic acids, nerve gas agents and other applications.

Investigation by theoretical quantum mechanical methods, of reactions of molecules on semiconductor surfaces leading to imprinting of molecular structure on the surfaces.

Electronic structure calculations on highly excited states of molecules, Rydberg states, autoionizing states.

Development and applications of theoretical methods for investigations of structure and processes in excited and highly excited states of small molecules.

Theoretical study of functionalized carbon nanohorns and fullerene hybrids.

### **TEACHING ACTIVITIES**

- 9-12/2002 Acting Laboratory Instructor, Organic Chemistry, Chemistry Department, University of Toronto,
- 9-12/1987 Sessional Lecturer at the Chemistry Department, Carleton University
- 9/1973-5/1978 Teaching Assistant at the Chemistry Department, University of Toronto, Toronto, Canada.

### **EXTERNAL FUNDING**

- (i) Member of team (I.D. Petsalakis, G. Theodorakopoulos and N. Tagmatarchis coordinator ) involved in NANOHOST project (FP7-REGPOT-2007-1), 2008-2011
- (ii) FP7-PEOPLE- IRG-2008, 2008-2012 (coordinator)
- (iii) Greece-Slovakia joint research and technology project, 2005-2007 (coordinator)
- (iv) Scientist in charge of MCIF-EU, 2003-2004
- (v) NATO PST/CLG.978504 , 2002-2003
- (vi) Greece-Poland joint research and technology project 2001-2003, (project coordinator)
- (vii) INTAS 1999, 2000-2003, (project coordinator)
- (viii) HCM-EC-40, 1994-1995
- (ix) Participation in other NATO and GSRT bilateral collaboration projects

## HONORS & AWARDS

EC Human Capital and Mobility category 40 fellowship, 1/8/94 - 31/7/95, Marie Curie Fellow , National Research Council of Canada, Post-Doctoral (NATO) Fellowship, 1978-1980, National Research Council of Canada, post-Graduate Scholarship, 1975-78, University of Toronto Open fellowship, 1974-75, Ontario Scholar (1969).

## PUBLICATIONS

155 articles have been published in refereed international scientific journals with about 1876 citations to the published work ( ISI web of science, March of 2017).

Full list of publications:

[http://www.eie.gr/nhrf/institutes/tpci/cvs/cv-theodorakopoulos\\_list.pdf](http://www.eie.gr/nhrf/institutes/tpci/cvs/cv-theodorakopoulos_list.pdf)

## SELECTED RECENT PUBLICATIONS

- N.N. Lathiotakis, G. Theodorakopoulos and I.D. Petsalakis, Electron transfer through organic molecular wires: A theoretical study. Chem. Phys.Let. 667, 45-50 (2017).  
[DOI: 10.1016/j.cplett.2016.11.044](https://doi.org/10.1016/j.cplett.2016.11.044)
- I.S.K. Kerkines, N. N. Lathiotakis, G. Theodorakopoulos and I.D. Petsalakis, Tailoring the spacer type and length in push-pull chromophores. Insights from a systematic theoretical study, Chem. Phys. Let. 653, 178-183 (2016).  
[DOI: 10.1016/j.cplett.2016.04.072](https://doi.org/10.1016/j.cplett.2016.04.072)
- D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, Molecular logic gates based on benzo-18-crown-6 ether of styrylquinoline: a theoretical study, Phys. Chem. Chem. Phys. 18, 32132-32145, (2016).  
[DOI: 10.1039/c6cp06899e](https://doi.org/10.1039/c6cp06899e)
- I. D. Petsalakis, G. Theodorakopoulos, O. Buchman, R. Baer, "Applicability of Mulliken's formula for photoinduced and intramolecular charge-transfer energies", Chem. Phys. Let. 625, 98-103, (2015).  
[DOI: 10.1016/j.cplett.2015.02.040](https://doi.org/10.1016/j.cplett.2015.02.040)
- J.V. Gavette, I.D. Petsalakis, G. Theodorakopoulos, K.D. Zhang, Y. Yu and J. Rebek, Jr, The effects of hexafluoroisopropanol on guest binding by water-soluble capsule and cavitand hosts, Chem. Comm.51, 17604-17606 (2015).  
[DOI: 10.1039/c5cc06405h](https://doi.org/10.1039/c5cc06405h)
- I.D. Petsalakis, G. Theodorakopoulos and J. Whitten, Electronic structure and spectra of (Cu<sub>2</sub>O)(n)-H<sub>2</sub>O complexes, Phys. Chem. Chem. Phys. 17, 428-433 (2015).  
[DOI: 10.1039/c4cp04303k](https://doi.org/10.1039/c4cp04303k)

- B. Pappas, I. D. Petsalakis, G. Theodorakopoulos and J. Whitten, CI and DFT Studies of the Adsorption of the Nerve Agent Sarin on Surfaces, *J. Phys. Chem. C*, 23042-23048 (2014).  
[DOI: 10.1021/jp505258k](https://doi.org/10.1021/jp505258k)
- I. D. Petsalakis and G. Theodorakopoulos, Boronic Acid sensors for saccharides: A theoretical study. *Chem. Phys.Lett.* 586, 1-115 (2013).  
[DOI:10.1016/j.cplett.2013.09.025](https://doi.org/10.1016/j.cplett.2013.09.025)
- M. G. Sarwar, D. Ajami, G. Theodorakopoulos, I. D. Petsalakis, and J. Rebek, Jr, Amplified Halogen Bonding in a Small Space , *J. Amer.Chem.Soc.* communication 135,13672 (2013).  
[DOI: 10.1021/ja407815t](https://doi.org/10.1021/ja407815t)
- D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, D. Ajami and J. Rebek, Jr, Conformations and fluorescence of encapsulated stilbene, *J. Amer. Chem.Soc.*134, 4346-4354 (2012).  
[DOI: 10.1021/ja211164b](https://doi.org/10.1021/ja211164b)
- I.D.Petsalakis and G.Theodorakopoulos, Molecular orbital assistance in the design of intramolecular and photoinduced electron transfer systems, *Chem. Phys.Lett.*, 525-26,105-109 (2012).  
[DOI: 10.1016/j.cplett.2012.01.002](https://doi.org/10.1016/j.cplett.2012.01.002)
- D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, Dariush Ajami and Julius Rebek, Jr, Theoretical study of hydrogen bonding in homodimers and heterodimers of amide, boronic acid and carboxylic acid, free and in encapsulation complexes, *J. Amer. Chem.Soc.* 16977-16985, 133 (2011).  
[DOI: 10.1021/ja206555d](https://doi.org/10.1021/ja206555d)
- I. S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos and J. Rebek, Jr, Excited state intramolecular proton transfer in hydroxy oxime-based chemical sensors, *The J. Phys. Chem. A.* 115, 834-840 (2011).  
[DOI: 10.1021/jp1088433](https://doi.org/10.1021/jp1088433)
- D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a pi-extended TTF derivative, 25, 1196-11975 (2011).  
[DOI: 10.1039/c0cp02665d](https://doi.org/10.1039/c0cp02665d)
- D. Irimia, I. D. Petsalakis, G. Theodorakopoulos and M. H. M. Janssen, Coherent Oscillatory Femtosecond Dynamics in Multichannel Photodynamics of NO<sub>2</sub> Studied by Spatially Masked Electron Imaging, *J. Phys. Chem. A.* 114, 3157-3166 (2010).  
[DOI: 10.1021/jp909031p](https://doi.org/10.1021/jp909031p)
- I. S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos and W. Klopper, Low-lying absorption and emission spectra of pyrene, 1,6-dithiaprene, and

tetrathiafulvalene: A comparison between ab initio and time-dependent density functional methods, J. Chem. Phys. 131, 224315 (2009).

**DOI:** [10.1063/1.3271347](https://doi.org/10.1063/1.3271347)

Full list of publications:

[http://www.eie.gr/nhrf/institutes/tpci/cvs/cv-theodorakopoulos\\_list.pdf](http://www.eie.gr/nhrf/institutes/tpci/cvs/cv-theodorakopoulos_list.pdf)