CURRICULUM VITAE

Vasilios Raptis

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EDUCATION

- Ph.D. in Chemistry, National and Kapodistrian University of Athens (2004)
- M.Sc. in Polymer Science and its Applications, National and Kapodistrian University of Athens (2000)
- Diploma in Chemical Engineering, National Technical University of Athens (1994)

RESEARCH EXPERIENCE (highlights)

04/2021 – present:	Postdoctoral Researcher, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Greece
02/2016-12/2020:	Postdoctoral Researcher, Foundation for Research and Technology-Hellas, Greece
12/2014-11/2015:	Postdoctoral Researcher, National Centre for Scientific Research-Demokritos, Greece
09/2012-09/2014:	Postdoctoral Researcher, Imperial College London (Chemical Engineering Dpt), United Kingdom
09/2004-08/2007:	Postdoctoral Researcher, University of Ioannina, Greece

MAIN RESEARCH INTERESTS

- Molecular simulation of molecular liquids, polymer solutions and amorphous melts, crystalline polymers, solid state systems
- Development of novel force fields to use in molecular simulations
- Quantum mechanical (*ab initio*, Density Functional Theory) calculations for the study of molecular and solid-state systems
- Development of novel theoretical models and techniques at the nanoscale level
- Photovoltaic materials, polymers, associating liquids
- Complex systems

TEACHING EXPERIENCE (University level)

03/2008-08/2012:	Adjunct Lecturer (full time), University of Ioannina, Greece
10/2007-02/2009:	Adjunct Lecturer (part time), University of Western Macedonia, Greece

PROFESSIONAL AFFILIATIONS & ACTIVITIES

- Member of the Technical Chamber of Greece

SELECTED PUBLICATIONS

1. "Molecular Dynamics Simulation of Structure and Thermodynamic Properties of Poly(dimethylsilamethylene) and Hydrocarbon Solubility Therein: Toward the Development of Novel Membrane Materials for Hydrocarbon Separation", V. Raptis, I. G. Economou, D. N. Theodorou, J. Petrou and J. Petropoulos, Macromolecules, 37(3), 1102 (2004).
2. "Force field development for poly(dimethylsilylenemethylene) with the aid of *ab initio* calculations", V. Raptis and V. Melissas, The Journal of Physical Chemistry B, 110(30), 14929 (2006).
3. "New effective method for quantitative analysis of diffusion jumps, applied in molecular dynamics simulations of small molecules dispersed in short chain

systems", T. Raptis, V. Raptis and J. Samios, The Journal of Physical Chemistry B, 111(49), 13683 (2007).

4. "Molecular dynamics study of the local structure and diffusivity of partially miscible water/n-alcohols binary mixtures", C. Dimitroulis, E. Kainourgiakis, V. Raptis and J. Samios, Journal of Molecular Liquids, 205, 46 (2015).
5. "Optical-vibrational properties of the Cs_2SnX_6 (X = Cl, Br, I) defect perovskites and hole-transport efficiency in dye-sensitized solar cells", A. Kaltzoglou, M. Antoniadou, A. G. Kontos, C. C. Stoumpos, D. Perganti, E. Siranidi, V. Raptis, K. Trohidou, V. Psycharis, M. G. Kanatzidis, and P. Falaras, Journal of Physical Chemistry C 120, 11777 (2016).
6. "Theoretical aspects of a discrete-binding approach in quartz-crystal microbalance acoustic biosensing", V. Raptis, A. Tsortos and E. Gizeli, Physical Review Applied, 11, 034031 (2019).