Publication list of Dr. Vasilios Raptis

1. PhD Thesis

"Calculation of structural, thermodynamic and hydrocarbon-transport properties of silicon-containing polymers *via* molecular simulation" (in Greek) Department of Chemistry, National and Kapodistrian University of Athens, 2004.

2. Publications in peer-reviewed journals

1. Raptis, V.; Dimitroulis, C.; Raptis, T. "Just type polyana and press Enter: a post-processing application designed with simplicity of use in mind" *Mol. Simulat.* **2019**, DL_POLY's 25th anniversary special issue, DOI:10.1080/08927022.2019.1603379 (online: 17 April 2019).
2. Raptis, V.; Tsortos, A.; Gizeli, E. "Theoretical aspects of a discrete-binding approach in QCM-D acoustic biosensing ", *Phys. Rev. Appl.* **2019**, 11, 034031.
3. Rahman, S.; Lobanova, O.; Jiménez-Serratos, G.; Braga, C.; Raptis, V.; Müller, E. A.; Jackson, G.; Avendaño, C.; Galindo, A. "SAFT-γ Force Field for the Simulation of Molecular Fluids. 5. Hetero-Group Coarse-Grained Models of Linear Alkanes and the Importance of Intramolecular Interactions" *J. Phys. Chem. B*, **2018**, *122*, 9161-9177.
4. Idrissi, A.; Marekh, B. A.; Barj, M.; Miannay, F. A.; Takamuku, T.; Raptis, V.; Samios, J.; Jedlovszky "Local structure of dilute DMSO solutions, as seen from molecular dynamics simulations" *J. Chem. Phys.* **2017**, *146*, 234507.
5. Elpidoforou, N.; Skarmoutsos, I.; Kainourgiakis, E.; Raptis, V.; Samios, J. "Local structure and translational dynamics of NMF (N-methylformamide)–DMF (N,N-dimethylformamide) mixtures, via molecular dynamics simulation" *J. Mol. Liq.* **2017**, *226*, 16-27.
6. Kaltzoglou, A.; Antoniadou, M.; Kontos, A.; Stoumpos, K.; Perganti, D.; Siranidi, E.; Raptis, V.; Trohidou, K.; Psycharis, V.; Kanatzidis, M.; Falaras, P. "Optical-vibrational properties of the Cs_2SnX_6 (X = Cl, Br, I) defect perovskites and hole-transport efficiency in dye-sensitized solar cells" *J. Phys. Chem. C*, **2016**, *22*, 11777-11785.
7. Tegou, E.; Magana, M.; Katsogridaki, A.-E.; Ioannidis, A.; Raptis, V.; Jordan, S.; Chatzipanagiotou, S.; Chatzandroulis, S.; Ornelas, C.; Tegos, G. P. "Terms of endearment: Bacteria meet graphene nanosurfaces" *Biomaterials*, **2016**, *89*, 38-55.
8. Kaltzoglou, A.; Antoniadou, M.; Perganti, D.; Siranidi, E.; Raptis, V.; Trohidou, K.; Psycharis, V.; Kontos, A. G.; Falaras, P. "Mixed-halide $Cs_2SnI_3Br_3$ perovskite as low resistance hole-transporting material in dye-sensitized solar cells" *Electrochim. Acta*, **2015**, *184*, 466-474.
9. Dimitroulis, C.; Raptis, T.; Raptis V. E. "POLYANA - A tool for the calculation of molecular radial distribution functions based on Molecular Dynamics trajectories" *Comput. Phys. Commun.* **2015**, *197*, 220-226.
10. Dimitroulis, C.; Kainourgiakis, E.; Raptis, V. E.; Samios, J. "Molecular dynamics study of the local structure and diffusivity of partially miscible water/n-alcohols binary mixtures" *J. Mol. Liq.*, **2015**, *205*, 46-53.
11. Raptis, T. E.; Raptis, V. E.; Samios, J. "Quantitative study of diffusion jumps in atomistic simulations of model gas – polymer systems" *Mol. Phys.*, **2012**, *110*, 1171-1178.
12. Raptis, T. E.; Raptis, V. E.; Samios, J. "A new effective method for quantitative analysis of diffusion jumps, applied in Molecular Dynamics simulations of small molecules dispersed in short chain systems" *J. Phys. Chem. B* **2007**, *111*, 13683-13693.

13. Makrodimitri, Z. A.; Raptis, V. E.; Economou, I. G. "Molecular Dynamics Simulation of Structure, Thermodynamic and Dynamic Properties of Poly(dimethylsilamethylene), Poly(dime-thylsilatrimethylene) and their Alternating Copolymer". *J. Phys. Chem. B*, **2006**, *110*, 16047-16058.
14. Raptis, V. E.; Melissas, V. S. "Force field development for poly(dimethylsilylene-methylene), with the aid of ab initio calculations". *J. Phys. Chem. B*. **2006**, *110*, 14929.
15. Economou, I. G.; Raptis, V. E.; Melissas, V. S.; Theodorou, D. N.; Petrou, J.; Petropoulos, J. H. "Molecular simulation of structure, thermodynamic and transport properties of polymeric membrane materials for hydrocarbon separation" *Fluid Phase Equilibria*, **2005**, *228–229*, 15-20
16. Alentiev, A.; Economou, I. G.; Finkelshtein, E.; Petrou, J.; Raptis, V. E.; Sanopoulou, M.; Soloviev, S.; Ushakov, N.; Yampolskii, Y. "Transport properties of silmethylene homopolymers and random copolymers: experimental measurements and molecular simulation" *Polymer*, **2004**, *45*, 6933-6944.
17. Raptis, V. E.; Economou, I. G.; Theodorou, D. N.; Petrou, J.; Petropoulos, J. H. "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" *Macromolecules*, **2004**, *37*, 1102-1112.

3. Conference papers (peer reviewed)

1. Raptis, V.; Harmandaris, V. "Properties of poly(lactate) acid chains *via* multiscale dynamic simulations using atomistic and coarse-grain models", 12th Panhellenic Scientific Conference in Chemical Engineering, Athens, Greece, May 29-31, **2019**
2. Maragkaki, A.; Sampathianakis, I.; Katrini, K.; Michalodimitraki, E.; Gryparis, C.; Raptis, V.; Power, A.; Lolos, T.; Tsobanidis, C.; Harmandaris, V.; Velonia, K.; Manios,T. "Bio-waste to Bio-plastic (B2B): Production of Compostable Bio-plastics from Food Waste" Proceedings (MDPI), **2019**, *30* (1), 47.
3. Rahman, S.; Braga, C.; Lobanova, O.; Raptis, V.; Galindo, A.; Jackson, G. and Müller, E. A. "The Importance of Intra- and Inter-Molecular Interactions in the Development of Coarse-Grained Models for Chain Fluids Using SAFT-γ Mie in Molecular Simulations" AIChE Annual Meeting, San Francisco, USA, November 3-8, **2013**
4. Economou, I. G.; Raptis, V. E.; Theodorou, D. N.; Petrou, J. and Petropoulos, J. H. «Novel Polymer Membrane Design for Hydrocarbon Separation Through Molecular Simulation», AIChE Annual Meeting, San Francisco, California, USA, November 16-21, **2003**

4. Preprints

1. Raptis, V.: "COVID-19: Escape routes from the Symplegades of hygienic crisis and economic meltdown" JMIR preprints, 2020, DOI: 10.2196/preprints.20022 (publication date: 9 May **2020**).
2. Raptis, T. E.; Raptis V.: "Understanding coil-to-globule transition of polymers with the aid of a novel cluster analysis technique", arXiv preprint, 2013, arXiv: 1307.7366 (publication date: 28 July 2013; revision date: 20 November **2013**).
3. Raptis, T. E.; Raptis V.: "A novel method of cluster analysis and applications thereof in sample molecular simulations", arXiv preprint, 2013, arXiv: 1306.3460 (publication date: 14 June **2013**)