RESEARCH INTERESTS

Molecular simulation of matter. Development of classical molecular models based on *Ab Initio* quantum mechanical calculations. Chemical Kinetics calculations with the use of quantum mechanical methods

ACADEMIC STUDIES

- PhD, Department of Chemistry, National and Kapodistrian University of Athens, 2004. (Research work performed at the Molecular Modelling of Materials Laboratory, Institute of Physical Chemistry, NCSR Demokritos)
- Msc., Polymer Science with Applications" Department of Chemistry, National and Kapodistrian University of Athens, 2000
- Chem. Eng. Diploma, School of Chemical Engineering, NTUA, Athens, 1994

OCCUPATION

Post-doctoral researcher. Department of Chemistry, University of Ioannina, 2004 – today

PUBLICATIONS

1. Makrodimitri, Z. A.; Raptis, V. E.; Economou, I. G. "Molecular Dynamics Simulation of Structure, Thermodynamic and Dynamic Properties of Poly(dimethylsilamethylene), Poly(dimethylsilatrimethylene) and their Alternating Copolymer" J. Phys. Chem. B, 2006, 110, 16047.
2. 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.
3. 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 Equilib., 2005, 228 – 229, 15.
4. Alentiev, A.; Economou, I. G.; Finkelshtein, E.; Petrou, J.; Raptis, V. E.; Sanopoulou, M.; Soloviev, S.; Ushakov, N.; Yampolskii, Y. ""Transport properties of silmethylene homo-polymers and random copolymers: experimental measurements and molecular simulation" Polymer, 2004, 45, 6933-6944.
5. 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.

INTERNATIONAL CONFERENCES

1. Papavasileiou, K. D.; Tzima, T. D.; Raptis, V. E.; Melissas, V. S., "An ab initio dynamics study of the CH 2Cl 2 + OH reaction" 19 th International Symposium on Gas Kinetics, Orléans, France, 22 – 27 July, 2006.
2. I. G. Economou , V. E. Raptis, D. N. Theodorou , J. Petrou and J. H. Petropoulos, "Molecular Simulation of Structure, Thermodynamic and Transport Properties of Polymeric Membrane Materials for Hydrocarbon Separation" 10 thInternational Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird, Utah, USA, 16 – 21 May, 2004.
3. I. G. Economou , V. E. Raptis, D. N. Theodorou , J. Petrou and J. H. Petropoulos, "Novel Polymer Membrane Design for Hydrocarbon Separation Through Molecular Simulation" AIChE Annual Meeting, Session 460, San Francisco, California, USA, 16 – 21, November 2003.
4. V. E. Raptis, I. G. Economou, D. N. Theodorou, J. Petrou and J. H. Petropoulos, "Molecular Modelling of Structure, Thermodynamic, and Transport Properties of Poly(dimethylsilamethylene) – Light Hydrocarbon Systems" 20 th European Seminar on Applied Thermodynamics, Lahnstein, Germany, 9 – 12, October 2003.
5. V. E. Raptis, V. S. Melissas, I. G. Economou, D. N. Theodorou, M. Sanopoulou, J. Petrou and J. H. Petropoulos, E. Sh. Finkelshtein, A. Alentiev and Y. P. Yampolskii , "Development of novel polymeric membranes for natural gas hydrocarbon separation through experimental measurements, quantum mechanics, molecular simulation and macroscopic modelling" 19th European Seminar on Applied Thermodynamics , Santorinh, Greece , 6 – 10 September, 2002.
6. V. E. Raptis, E. G. Hatzopoulou, V. S. Melissas, I. G. Economou, D. N. Theodorou, "Conformational aspects of poly(dimethylsilaethylene) based on quantum chemistry calculations" 2nd International Conference of the Chemical Societies of the South-Eastern European Countries, Chalkidiki, Greece , 6 – 9 June 2000.