



Andreas Koutselos

Associate Professor of Physical Chemistry



Education

B.Sc. in Chemistry, National and Kapodistrian University of Athens, Greece, (1981).
 Ph.D. in Physical Chemistry, Brown University, Providence RI. USA, (1986).
 Post Doctoral studies at Stanford University, Stanford, CA. USA, (1987) and
 Boston College, Boston, MA. USA, (1989).



Research Field of Interest

Dynamics and transport of chemical systems through stochastic and kinetic theory calculations, as well as, through Molecular Dynamics simulations. Special systems consist of ions moving in fluids under the action of an electric field and chemical reacting systems constrained out of equilibrium.



Teaching

Undergraduate: 613 Physical Chemistry III

Graduate: Physical Chemistry, Statistical Mechanics



Selected Papers

- "Correlation and Prediction of Dispersion Coefficients for Isoelectronic Systems", A. D. Koutselos and E. A. Mason, *J. Chem. Phys.* **85**, 2154, (1986).
- "Interaction Universality and Scaling Laws for Interaction Potentials between Closed - Shell Atoms and Ions", A. D. Koutselos, E. A. Mason and L. A. Viehland, *J. Chem. Phys.* **93**, 7125, (1990).
- "Model Molecular Hamiltonians ", A. D. Koutselos and U. Mohanty, *Physica*, **A166**, 99, (1990).
- "Generalized Einstein Relations for Ions in Molecular Gases", A. D. Koutselos and E. A. Mason, *Chem. Phys.* **153**, 351, (1991).
- "Thermodynamic Steady State Laws for Nonlinear Chemical Systems Far from Equilibrium", A. D. Koutselos, *Phys. Let. A.* **180**, 103, (1993).
- "Steady State Thermodynamics for Homogeneous Chemical Systems", A. D. Koutselos, *J. Chem. Phys.* **101**, 10866, (1994).
- "Molecular Dynamics Simulation of Gaseous Ion Motion in Electrostatic Fields", A. D. Koutselos, *J. Chem. Phys.* **102**, 7216, (1995).
- "Velocity Correlation functions, Fickian and Higher Order Diffusion Coefficients for Ions in Electrostatic Fields via Molecular Dynamics Simulation", A. D. Koutselos, *J. Chem. Phys.* **104**, 8442, (1996).
- "Dynamic Properties and Third Order Diffusion Coefficients of Ions in Electrostatic Fields", A.

D. Koutselos, J. Chem. Phys. **106**, 7117, (1997).

"Ion Dynamics in Electrostatic Fields", A. D. Koutselos, J.Phys.B: At. Mol. Opt. Phys. **32**, 1225, (1999)

"Third Order Transport Properties of Ions in Electrostatic Fields", A. D. Koutselos, J. Chem. Phys. **110**, 3256, (1999).

"Third Order Transport Properties from the Moment Solution Boltzmann Equation for Gaseous Ions in Electrostatic Fields", A. D. Koutselos, Chem. Phys. **270**, 165 (2001).

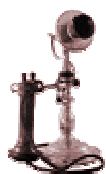
"Molecular dynamics simulation of ion transport in moderately dense gases in an electrostatic field", G. Balla and A. D. Koutselos, J. Chem. Phys. **119**, 11374 (2003).

"Transport properties of diatomic ions in moderately dense gases in an electrostatic field", A. D. Koutselos and J. Samios, Pure Appl. Chem. **76**, 223 (2004).

"Nonequilibrium Molecular Dynamics Simulation of Diatomic Ions in Supercritical Gases in an Electrostatic Field". N. D. Margetis and A. D. Koutselos, *"Lecture Series on Computer and Computational Sciences"*, **1**, 341 (2004), Eds T. Simos and G. Maroulis.

"Third-Order Transport Properties of Ion-Swarms from Mobility and Diffusion Coefficients", A. D. Koutselos, Chem. Phys. **315**, 193 (2005).

"Mixed Quantum-Classical Molecular Dynamics Simulation of Vibrational Relaxation of Ions in an Electrostatic Field", A. D. Koutselos, J. Chem. Phys. **125**, 244304 (2006).



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