



Andreas D. Koutselos

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, (1988).

Visiting Scholar, Brown University RI. USA, (1990) and (1994), Van 't Hoff Institute, UvA, Holland (2006).

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 electromagnetic field and chemical reacting systems.

Teaching

Undergraduate: 514 Physical Chemistry II, in the past 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).

"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).

"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).

"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).

"Transport and dynamic properties of O_2^+ ($X^2\Pi_g$) in Kr under the action of an electrostatic field: Single or multiple potential energy surface treatment", A. D. Koutselos, J. Chem. Phys. **134**, 194301 (2011).

"Dynamics and drift motion of O_2^- in supercritical argon", Andreas D. Koutselos, Jannis Samios, J. Mol. Liq. **205**, 115 (2015).

"Molecular dynamics simulation for the dynamics and kinetics of folding peptides in the gas phase", I. Litinas and A. Koutselos. J. Phys. Chem. A. **119**, 12935, (2015).

"Dynamics of flexible peptides under the action of an electrostatic field in the gas phase", Iraklis Litinas and Andreas D. Koutselos, J. Mol. Liq. **245**, 115 (2017).

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