Jiří Kolafa – CV (October 20, 2022)

Contacts

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Personal Data

- Born September 20, 1958 in Jičín, East Bohemia, Czechoslovakia
- Married (1984), two children (1985 and 1989)

Education and employment

- 1977–1982 Faculty of Mathematics and Physics, Charles University, Prague
- 1982 M.S. and RNDr. in Mathematical Physics (supervisor: Roman Kotecký)
- 1983–1985 Department of Mathematical Physics, Charles University, Prague
- 1985–1989 PhD. in Physical Chemistry, Institute of Chemical Process Fundamentals, Academy of Sciences, Prague (supervisor: Ivo Nezbeda)
- 1989–2001 Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic, Prague
- 2001–now Department of Physical Chemistry, Institute of Chemical Technology, Prague
- 2004 Associate Professor
- 2010 Professor of Physical Chemistry

Temporary positions

- 1991–1995 Lindø Center for Applied Mathematics, Odense University, Denmark – Prof. John W. Perram. Total 3 years, molecular dynamics simulations of macromolecules
- 1991–2001 Department of Chemistry, Northwestern University, Evanston, Illinois, USA – Prof.
- Mark Ratner. Total 8 months, molecular dynamics simulations of macromolecules and molten salts
- 1996 Department of Mathematics & Statistics, University of Guelph, Guelph, Ontario, Canada – Prof. W. R. Smith, 6 months, global phase diagrams

Current research interests

- Nucleation from vapor, clusters in vacuum
- Ionic solutions, solubility, chemical potential of crystals
- Water and ice from the point of view of statistical thermodynamics and simulation
- Methodology of molecular simulations, MD integrators, polarizable models, charge scaling, force field development

Former fields of activity

- Simple models of fluids like hard spheres, diagrammatic techniques, integral equations
- Ionic liquids
- Global phase diagrams

Scientometrics

- 100 research papers (Web of Science, Oct 20, 2022)
- Times cited: 2,934 (total), 2,697 (without self-itations)
- H-index: 29
- ORCID: 0000-0002-5096-7346
- ReseacherID: B-7513-2008

Teaching

- **Bc. courses:** Physical chemistry (A, B, and colloid chemistry, of microcosmos), Computational chemistry, Molecular Modeling and Simulation (for Technical University Liberec)
- **Mgr. courses:** Mathematics for Physical Chemistry, Statistical Thermodynamics and Molecular Modeling and Simulation
- **PhD. courses:** Molecular Modeling and Simulation

Other activities

- Chair of the Doctoral program board in Physical Chemistry

Scientific software

- **MACSIMUS**: Molecular modeling and simulation package, 140,000 lines of code and data
- **HSMD**: Highly optimized MD code for the hard sphere fluid, 4000 lines of code
- **NSK**: GUI-oriented software for phase equilibria and global phase diagrams, 10,000 lines of code

Educational software

- **SIMOLANT**: MC/MD simulation of a 2D system, for teaching physical chemistry and molecular simulations
- **Redlich–Kwong** equation of state, Java script applet

Five most cited papers

As of Web of Science (Oct 20, 2022)

1. Kolafa J and Nezbeda I: The Lennard-Jones fluid – an accurate analytic and theoretically-based equation of state, Fluid Phase Equil 100, 1 (1994), 249 citations
2. Kolafa J and Perram JW: Cutoff errors in the Ewald summation formulas for point-charge systems, Mol Simul 9, 351 (1992), 211 citations
3. Kolafa J and Nezbeda I: Monte-carlo simulations on primitive models of water and methanol, Mol Phys 61, 161 (1987), 169 citations
4. Kolafa J: Time-reversible always stable predictor-corrector method for molecular dynamics of polarizable molecules, J Comput Chem 25, 335 (2004), 156 citations
5. Kolafa J, Labík S and Malijevský A: Accurate equation of state of the hard sphere fluid in stable and metastable regions, Phys Chem Chem Phys 6, 2335 (2004), 126 citations

Ten recent papers

In the order of Web of Science (Oct 20, 2022)

1. Suchan J, Kolafa J and Slavíček P: Electron-induced fragmentation of water droplets: Simulation study, J Chem Phys 156, 144303 (2022)
2. Celný D, Klíma M and Kolafa J: Molecular dynamics of heterogeneous systems on GPUs and their application to nucleation in gas expanding to a vacuum, J Chem Theory Comput 17, 7397 (2021)
3. Hantal G, Kolafa J, Sega M and Jedlovszky P: Single-particle dynamics at the intrinsic surface of aqueous alkali halide solutions, J Phys Chem B 125, 665 (2021)
4. Hantal G, Horvath RA, Kolafa J, Sega M and Jedlovszky P: Surface affinity of alkali and halide ions in their aqueous solution: Insight from Intrinsic density analysis, J Phys Chem B 124, 9884 (2020)
5. Kolafa J: Pressure in molecular simulations with scaled charges. 1. Ionic systems, J Phys Chem B 124, 34 (2020)
6. Janek J and Kolafa J: Novel Gear-like predictor–corrector integration methods for molecular dynamics, Mol Phys 118, e1674937 (2020)
7. Kolafa J: Topological and real charge of Bjerrum defects in ices Ih and Ic, Mol Phys 118, e1705410 (2019)
8. Kolafa J: Free energy of classical molecular crystals by thermodynamic integration from a harmonic reference, J Chem Theory Comput 15, 68 (2019)
9. Smith WR, Nezbeda I, Kolafa J, Moučka F: Recent progress in the molecular simulation of thermodynamic properties of aqueous electrolyte solutions, Fluid Phase Equi 446, 19 (2018)
10. Moucka F, Kolafa J, Lisal M and Smith WR: Chemical potentials of alkaline earth metal halide aqueous electrolytes and solubility of their hydrates by molecular simulation: Application to CaCl2, antarcticite, and sinjarite, J Chem Phys 144, 222832 (2018)