Krzysztof Szalewicz

szalewic@udel.edu

Professional Preparation

1984	D.Sc., University of Warsaw
1977	Ph.D. (with honors, in Chemistry), University of Warsaw
1973	M.S. (with honors, in Chemistry), University of Warsaw

Appointments

1994-	Professor, Department of Physics and Astronomy, University of Delaware
2014,2015	Visiting Professor, Copernicus University, Torun (one month)
2009-2010	Visiting Professor of Astronomy, LAOG, Grenoble
2002-2003	Visiting Fellow, Princeton University
2002-	Member of Center for Molecular and Engineering Thermodynamics, UD
1996	ITAMP Visitor, Harvard-Smithsonian Center for Astrophysics, Harvard U.
1995	JILA Fellow, Joint Institute for Laboratory Astrophysics, NIST/University of Colorado
1993-	Joint Appointment at the Department of Chemistry and Biochemistry, UD
1990-1994	Associate Professor, Department of Physics and Astronomy, UD
1990-1992	Visiting Scientist, Department of Quantum Chemistry University of Uppsala, Sweden (several visits of a few weeks each)
1988-1990	Assistant Professor, Department of Physics and Astronomy, UD
1985-1987	Associate Research Scientist (a nontenure-track faculty position), Quantum Theory Project, Department of Physics, University of Florida
1982-1984	Visiting Scientist, Institute of Theoretical Physics, University of Cologne, Germany (several visits of a few weeks each)
1980-1982	Adjunct Research Assistant Professor, Quantum Theory Project, Departments of Physics and Chemistry, University of Florida
1978-1984	Assistant Professor, Department of Chemistry, University of Warsaw

Honors and Awards

2010-	Elected Member of International Academy of Quantum Molecular Science (IAQMS)
2006	PULPIT lecturer: a series of lectures at Cambridge U., University College London, U. Nottingham, Durham U.
2004	UD College of Arts & Science Outstanding Scholar Award
2001	AMPOL's Annual Achievement Award (AMPOL is the Americans of Polish Descent Cultural Society)
2001-	Member of the Franklin Institute (FI) Award Committee
2000-	Fellow of the American Physical Society
1979	Research Award of the Minister of Higher Education of Poland
1977-1984	Awards of the President of the University of Warsaw (4 times)
1971-1973	Research Scholarship, University of Warsaw

Research Interests

Current interests are focused on the phenomenon of weak intermolecular interactions. Such interactions determine structure and dynamics of molecular clusters, condensed phases, and biomolecular systems. Properties of such systems can be predicted if force fields (FFs) for nuclear motion are known. Such FFs can be computed from first principles using symmetry-adapted perturbation theory (SAPT) co-developed by our group and are relevant in several fields of physics, astrophysics, chemistry, metrology, and technology: (a) Calculation involving helium atoms were used to establish the newest standard of temperature; (b) Predictions of of structure, spectra, and scattering cross-sections help in interpretation of relevant mea-

surements and provide data needed to understand processes in interstellar molecular clouds; (c) Molecular simulation of liquids such as water are aimed at understanding mysterious properties of such systems; (d) Crystal structure predictions base on our FFs are expected assist pharmaceutical industry in finding polymorphic forms of drugs; (e) New generation of biomolcular FFs have the promise of transforming the field of simulations of biosystems and of materials modelling and design.

Recent Synergistic Activities

(a) Symmetry-adapted perturbation theory (SAPT) codes are distributed free of charge and are used by more than 900 research groups worldwide (http://www.physics.udel.edu/∼szalewic/SAPT/SAPT.html). Part of our group time is spent helping users with issues encountered when running SAPT. (b) Members of IAQMS work on awarding Academy medals to young scientists and organize congresses. (c) Members of the FI Award Committee work on popularization of science through Award Symposia, which draw a significant nonphysics audience, and other FI activities. (d) Organization of scientific meetings (e.g., ARO Workshops, ACS Symposium, Telluride Workshops, and "Water Festivals").

Selected Publications [over 270 refereed papers and a textbook, H-index: 73 (Google Scholar 84), one paper cited over 2200 times, 46 papers cited over 100 times (source: Web of Science).]

1. O. Fackler, B. Jeziorski, W. Kolos, H.J. Monkhorst, and K. Szalewicz "Accurate Theoretical β-Decay Energy Spectrum of Tritium Molecule and Its Neutrino Mass Dependence", Phys. Rev. Lett. **55**, 1388-1391 (1985).

2. B. Jeziorski, R. Moszynski, and K. Szalewicz "Perturbation theory approach to intermolecular potential energy surfaces of van der Waals complexes", Chem. Rev. **94**, 1887-1930 (1994).

3. A.J. Misquitta, B. Jeziorski, and K. Szalewicz "Dispersion energy from density-functional theory description of monomers", Phys. Rev. Lett. **91**, 033201:1–4 (2003).

4. R. Bukowski, K. Szalewicz, G. C. Groenenboom, and A. van der Avoird "Predictions of the Properties of Water from First Principles", Science **315**, 1249–1252 (2007).

5. R. Podeszwa, B. M. Rice, and K. Szalewicz "Predicting structure of molecular crystals from first principles", Phys. Rev. Lett. **101**, 115503:1–4 (2008).

6. K. Patkowski, V. Spirko, and K. Szalewicz "On the Elusive Twelfth Vibrational State of Beryllium Dimer", Science **326**, 1382-1384 (2009).

7. P. Jankowski, A. R. W. McKellar, and K. Szalewicz "Theory untangles high-resolution infrared spectrum of the *ortho*H_2-CO van der Waals complex", Science **336**, 1147–1150 (2012).

8. S. Chefdeville, T. Stoecklin, C. Naulin, P. Jankowski, K. Szalewicz, A. Faure, M. Costes, and A. Bergeat "Experimental and theoretical analysis of low-energy CO + H_2 inelastic collisions", Ap. J. Lett. **799**, L9:1-4 (2015).

9. M. Przybytek, W. Cencek, B. Jeziorski, and K. Szalewicz "Pair potential with submillikelvin uncertainties and nonadiabatic treatment of the halo state of the helium dimer", Phys. Rev. Lett. **119**, 123401:1–6 (2017).

10. M. Shahbaz and K. Szalewicz "Dispersion Energy from Local Polarizability Density", Phys. Rev. Lett. **122**, 213001:1-6 (2019).

11. A. Jing, K. Szalewicz, and A. van der Avoird "Ammonia dimer: extremely fluxional but still hydrogen bonded", Nature Comm. **13**, 1470:1–8 (2022).

12. R. Nikhar and K. Szalewicz "Reliable crystal structure predictions from first principles", Nature Comm. **13**, 3095:1–9 (2022).