Curriculum Vitae of Józef Adam Liwo

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Current positions:

- Full Professor and Head of Laboratory of Molecular Modeling, Faculty of Chemistry, University of Gdańsk, Gdańsk, Poland.
- KIAS Scholar, Korea Institute for Advanced Study, Seoul, Rep. of Korea.

Education, scientific degrees and titles:

- 2001: Professor of Chemical Sciences (title received from the President of the Republic of Poland after approval by the Central Committee for Scientific Degrees and Titles).
- 1997: Habilitation (Physical and Theoretical Chemistry) Faculty of Chemistry, University of Gdańsk, Poland.
- 1989: PhD (Physical and Theoretical Chemistry) Faculty of Mathematics, Physics, and Chemistry Chemistry, University of Gdańsk, Poland.
- 1983: MSc (Chemistry, with honors) Faculty of Mathematics, Physics, and Chemistry, University of Gdańsk, Poland. The curriculum included extended program in math.

Training:

- 1990-1992, 1994, Postdoctoral Associate, Department of Chemistry and Chemical Biology, Cornell University (supervisor: H.A. Scheraga).

Employment:

- 1983-present Faculty of Chemistry, University of Gdańsk; tenured full professor since 2001; member of the Faculty Council since 1997; director of the Laboratory of Molecular Modeling since 1999.
- 2014-present: Korea Institute for Advanced Study (KIAS), Seoul, Republic of Korea; KIAS Scholar.
- 2003-2010 Senior Research Associate, Dep. of Chemistry and Chemical Biology, Cornell University (H.A. Scheraga group).
- 2001-2003 Vice-Director for Scientific Affairs, Academic Computer Center in Gdańsk, TASK.
- several short-term employments on the visiting-scientist or visiting professor basis (Cornell University (USA), Mt. Sinai School of Medicine (USA), SUNY Upstate Medical Center (USA), University of Uppsala (Sweden), Beijing Institute of Technology (P.R. China) in years 1993-2015.

Organizational activity:

- 1998-present – Member of the Interdisciplinary Team of Mathematical Modeling at the Academic Computer Center in Gdańsk, TASK.
- 1998-2001 – President of the Scientific Council of the Academic Computer Center in Gdańsk, TASK.
- Co-organizer of 6 international conferences.

Professional Memberships:

- 2008-present: Member of the American Chemical Society.
- 2009-present: Member of the Biophysical Society.

- 2015-present: Member of the Polish Chemical Society.
- 2003-present: Member of the Scienfitic Society of Gdańsk.
- 2001-prsent: Member of the Polish Society of Computer Simulation.
- 2012-2015 Member of the Committee of Biochemistry and Biophysics of the Polish Academy of Sciences.

Honors and Awards:

- 2016 - medal of the Polish Committee of National Education.
- 2015 – Travel Award from Biophysical Society (presented on 59th National Biophysical Societ Meeting in Baltimore)
- 2013 – "Mistrz" (Master) subsidy for distinguished professors from the Foundation from Polish Science.
- 2013, 2006, 1999, 1993 - award from the Rector of the University of Gdansk for distinguished research.
- 2012 – Elected a member of the Committee of Biochemistry and Biophysics of the Polish Academy of Sciences.
- 2001, 1995, 1989 - Award as a team member from the Polish Minister of Education;
- 1998 – individual award from the Polish Minister of Education.

Publications:

245 original papers published, and 10 review articles, 7 original papers and 2 review articles in non-ISI journals, 12 book chapters, editor of 1 book. Number of citations excluding self-citations: 4834. **H-index: 43**.

Five most relevant publications in the last 5 years:

1. **A. Liwo**, A. K. Sieradzan, A. G. Lipska, C. Czaplewski, I. Joung, W. Żmudzińska, A. Hałabis, S. Ołdziej. A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. III. Determination of scale-consistent backbone-local and correlation potentials in the UNRES force field and force-field calibration and validation. *J. Chem. Phys.*, **2019**, 150, 155104
2. A.K. Sieradzan, M. Makowski, A. Augustynowicz, **A. Liwo**. A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. I. Backbone potentials of coarse-grained polypeptide chains. *J. Chem. Phys.*, **2017**, 146, 124106 (corresponding author).
3. A. Karczyńska, C. Czaplewski, P. Krupa, M. Mozolewska, K. Joo, J. Lee, A. Liwo. Ergodicity and model quality in template-restrained canonical and temperature/Hamiltonian replica exchange coarse-grained molecular dynamics simulations of proteins. *J. Comput. Chem.*, **2017**, 38, 2730–27 (corresponding author).
4. M.A. Mozolewska, P. Krupa, B. Zaborowski, **A. Liwo**, J. Lee, K. Joo, C. Czaplewski. Use of restraints from consensus fragments of multiple server models to enhance protein structure prediction capability of the UNRES force field. *J. Chem. Inf. Model.*, **2016**, 56, 2263-2279 (corresponding author).
5. B. Zaborowski, D. Jagieła, C. Czaplewski, A. Hałabis, A. Lewandowska, W. Żmudzińska, S. Ołdziej, A. Karczyńska, C. Omieczynski, T. Wirecki, **A. Liwo**. A maximum-likelihood approach to force-field calibration. *J. Chem. Inf. Model.*, **2015**, 55, 2050–2070 (corresponding author).

Research interests: coarse graining, molecular dynamics algorithms, statistical mechanics, generalized-ensemble sampling, molecular modeling, quantum mechanics, chemometry.

Research support (with role as PI): currently 1 research grant from Polish National Science Center (NCN), 5 major grants from the Polish government in years 1996-2017, Mistrz subsidy from the Foundation for Polish Science (2014-2016), 2 Collaborative Linkage Grants (CLG) from NATO (1999-2004), several small grants to support graduate students.

Teaching and mentoring: Present: 1 obligatory course (Theoretical Chemistry; course director) for M.Sc. students, 2 courses for Chemistry majors (Numerical Methods in Chemistry and Programming in C and FORTRAN), 2 lectures for graduate students (Protein Structure and Energetics and Molecular Simulations in Chemistry). In the past: General and Inorganic Chemistry lab and recitation classes (as T.A.), Informatics in Chemistry (lectures and lab classes), Molecular Modeling (lectures and lab classes).

11 graduate students, 11 undergraduate students and 1 postdoc mentored.