

CURRICULUM VITAE

Name: Titus Adrian
Family name: Beu
Date / place of birth: 04.05.1958, Cluj-Napoca, Romania
Nationality: Romanian
Scientific title: Dr.
Present position: Professor
Address (office): University „Babeş-Bolyai“, Faculty of Physics,
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Languages: English and German – very good / fluent, French - average

Education

Institution	Period	Programme / Degree
German School, Cluj-Napoca	09.1965 – 06.1973	Primary and junior high school
Mathematics-Physics High School and “Emil Racoviță” High School, Cluj-Napoca	09.1973 – 06.1977	High school / Baccalaureate
University “Babeş-Bolyai“, Faculty of Physics, Cluj-Napoca	09.1978 – 06.1982	Bachelor, Degree with Honors
University of Bucharest, Faculty of Physics, Bucharest	09.1982 – 06.1983	Master (Specialization) in Optics-Spectroscopy-Plasma-Lasers
University “Babeş-Bolyai“, Faculty of Physics, Cluj-Napoca	09.1986 – 05.1990	PhD in Physics: “Theoretical Study of Tokamak Impurities”

Professional career

Institution	Period	Position	Department
Institute for Nuclear Power Reactors, Pitești, Romania	09.1983 – 09.1985	Staff researcher	Department of Computer Science
Institute of Isotopic and Molecular Technology, Cluj-Napoca	09.1985 – 09.1987	Staff researcher	Department of Molecular Physics
University “Babeş-Bolyai“, Faculty of Physics, Cluj-Napoca	09.1987 – 09.1990	Assistant Professor	Department of Theoretical and Computational Physics
University “Babeş-Bolyai“, Faculty of Physics, Cluj-Napoca	09.1990 – 09.1996	Lecturer	Department of Theoretical and Computational Physics
University “Babeş-Bolyai“, Faculty of Physics, Cluj-Napoca	09.1996 – 09.2001	Associate Professor	Department of Theoretical and Computational Physics
University “Babeş-Bolyai“, Faculty of Physics, Cluj-Napoca	09.2001 –	Professor	Department of Theoretical and Computational Physics

Visiting scientist/professor positions abroad

Institution	Period	Funding	Position
Max-Planck-Institut für Strömungsforschung, Göttingen, Germany	11.1992 – 02.1993	EU Tempus	Visiting scientist
	10.1993 – 12.1993	EU Cost	Visiting scientist
	08.1994 – 10.1994	Max-Planck Foundation	Visiting scientist
Institute of Physical and Chemical Research (RIKEN), Wako-shi, Japan	04.1994 – 04.1994	RIKEN	Visiting scientist
	11.1994 – 11.1995		
	04.1997 – 10.1997		
	07.1998 – 09.1998		
	07.1999 – 08.1999		
Max-Planck-Institut für Strömungsforschung, Göttingen, Germany	11.1999 – 12.1999	Alexander von Humboldt Foundation	Visiting scientist
	04.2000 – 05.2000		
	11.2000 – 12.2000		
	07.2001 – 08.2001		
	11.2001 – 12.2001		
	02.2002 – 03.2002		
	08.2002 – 09.2002		
	11.2002 – 12.2002		
	02.2003 – 02.2003		
	08.2003 – 10.2003		
	02.2004 – 02.2004		
11.2004 – 11.2004			
Tokyo Institute of Technology, O-okayama, Tokyo, Japan	02.2004 – 08.2004	Tokyo Institute of Technology	Visiting Professor
	11.2008 – 11.2008		

National / international research programs / projects

Project / program	Period	Position
Alexander von Humboldt Stiftung, Germany: Program „Forschungskoooperation - Institutspartnerschaft“	1999 – 2004	Partner
CNCSIS: „Calculations of structure and vibrational dynamics for carbon nanostructures and molecular clusters“	2002 – 2005	Project leader
CERES: „Modelling ultra-short laser pulses in gases and atmosphere“	2003 – 2005	Partner
CEEX: „Transport and structuring processes at micro/nanometric scale in biomedicine and material science“	2005 – 2008	Team leader
CNCSIS: „Calculation of structural and dynamic properties for clusters, nanostructures and nanodevices“	2006 – 2009	Project leader
PN II PCE: „Quantum dot lattices and carbon nanostructures“	2007 – 2010	Partner
PN II PCE: „Modelling the carbon nanostructures and their functionalized derivatives“	2007 – 2010	Partner
COOPBIL Hungary: „Computer simulation and theoretical study of amorphous thin films and carbon and selenium nanostructures“	2008 – 2010	Team leader
PN-II-ID – PCCE: “Biofunctional particles for new imagery, sensing, diagnostic, and molecular therapy methodologies“	2011 – 2013	Team leader
PN-III-P4-ID-PCE-2016-0474: “Computational design of cationic polymers as gene delivery vectors“	2017 – 2019	Project leader

Research field

Theoretical and computational studies of nanostructures, soft matter, and complex biomolecular systems

Current research topics

- Force fields and molecular dynamics of biopolymers for gene delivery.
- Solvation/crystallization of calcites and CO₂ sequestration.
- Nanofluidics. Transport through carbon nanotubes and ion channels

Selected books

1. **T. A. Beu**,
“Introduction to Numerical Programming: A Practical Guide for Scientists and Engineers Using Python and C/C++”
(CRC Press / Taylor & Francis, 2015) 674 pp., ISBN 9781466569676.
2. O. G. Piringer, **T. A. Beu**,
“Transport Equations and Their Solutions”, in Plastic Packaging: Interactions with Food and Pharmaceuticals,
Second Edition, Editors O.-G. Piringer and A.L. Baner
(Wiley-VCH, Weinheim, New York, 2008) pp. 195-246.
3. **T. A. Beu**,
“Numerical solutions of the diffusion equation”, in Plastic Packaging Materials for Food: Barrier Function, Mass
Transport, Quality Assurance, and Legislation, Editors O.-G. Piringer and A.L. Baner
(Wiley-VCH Verlag GmbH, Weinheim, 2007) pp. 221-238.
4. **T. A. Beu**, "Numerical Calculus in C, Third Edition", (MicroInformatica, Cluj-Napoca, 2004) 372 pp. (in Romanian) .
ISBN 973-9443-92-3.

Relevant journal articles

1. **T. A. Beu**, A. Bende, A.-A. Farcaş, “Calculations of electron transfer in the tris[4-(2-thienyl)phenyl]amine–C70
donor-acceptor system”, Chem. Phys. Lett., 754 (2020) 137654, DOI: 10.1016/j.cplett.2020.137654.
2. **T. A. Beu**, A. E. Ailenei, R. I. Costinaş, “Martini Force Field for Protonated Polyethyleneimine”, J. Comput. Chem.
41 (2020) 349-361, DOI: 10.1002/jcc.26110.
3. A.-A. Fracaş, **T. A. Beu**, A. Bende, “Light-induced spin transitions in Ni(II)-based macrocyclic-ligand complexes: A
DFT study”, J Photochem. & Photobiol. A: Chem. 376 (2019) 316-323, DOI: 10.1016/j.jphotochem.2019.03.027.
4. **T. A. Beu**, A. E. Ailenei, A. Farcaş, “Atomistic and Coarse-Grained Modeling of Polyethyleneimine”, Chem. Phys.
Lett., 714 (2019) 94-98, DOI: 10.1016/j.cplett.2018.10.071.
5. **T. A. Beu**, A. E. Ailenei, A. Farcaş, “CHARMM Force Field for Protonated Polyethyleneimine”, J. Comput. Chem. 39
(2018) 2564–2575, DOI:10.1002/jcc.25637.
6. **T. A. Beu**, A. Farcaş, CHARMM force field and molecular dynamics simulations of protonated polyethylenimine,
J. Comput. Chem. 38 (2017) 2335–2348, DOI: 10.1002/jcc.24890.
7. **T. A. Beu** and A. Farcaş, “Tight-binding normal mode analysis of suspended single-wall carbon nanotubes”, EPL
113 (2016) 37004.
8. S. Höfner, A. Acocella, S. C. Pop, T. Narumi, K. Yasuoka, **T. Beu**, and F. Zerbetto, “GPU-Accelerated Computation
of Electron Transfer”, J. Comput. Chem. 33 (2012) 2351–2356.
9. **T. A. Beu**, “Molecular dynamics simulations of ion transport through carbon nanotubes. II. Structural effects of
the nanotube radius, solute concentration, and applied electric fields”, J. Chem. Phys. 135 (2011) 044515-11.
10. **T. A. Beu**, “Molecular dynamics simulations of ion transport through carbon nanotubes. III. Influence of the
nanotube radius, solute concentration, and applied electric fields on the transport properties”, J. Chem. Phys. 135
(2011) 044516-9.

Scientometric indicators

WoS ResearcherID: A-9524-2011, Scopus ID: 6701410591, UEFISCDI ID: U-1700-028G-2078

Google Scholar (GS)

Total number of cites (GS WoS):	898 754	Individual ISI Impact Factor / author:	66.0
Cites without self-cites (WoS):	661	Individual Article Influence Score / author:	24.6
Average citations / item (Wos):	13.2	Article Influence Score as main author:	40.2
h-index (GS WoS):	18 16	Cites / author:	322

Member in professional and academic bodies

- Expert of the Research Executive Agency, European Commission (2012-).
- Member of the Physics Commission, National Council for University Titles, Diplomas, and Certificates (2011-).
- Member of the Executive Committee, Santander Group of European Universities (2010-13).
- Vice-chair of the Physics Commission, National Council for University Titles, Diplomas, and Certificates (2011-12).
- Member of the National Council for Ethics, Ministry of Education and Research (2011-12).
- Member of the Natural Science Commission, National Research Council (2007-11).

Invited Professor

- Visiting Professor at Tokyo Institute of Technology, 2004.
- Invited speaker: University Osnabrück, 2001, Rheinisch-Westfälische Technische Hochschule Aachen, 2001, University Osnabrück, 2002, Tokyo Institute of Technology 2004 and 2008, University Rostock 2009, Technical University Graz 2011, Rice University (Houston) 2011, Kyoto University 2012.

Referee for international journals

- ACS Nano,
- Computational Materials Science,
- European Physical Journal B,
- European Physics Letters,
- Journal of Chemical Physics,
- Journal of Molecular Graphics and Modelling,
- Journal of Physical Chemistry,
- Journal of Physics: Condensed Matter,
- Langmuir,
- Nanotechnology,
- Theoretical Chemistry Accounts.

Teaching experience

- Quantum Mechanics (in Romanian, English, and German)
- Statistical Physics (in Romanian and German)
- Methods of Computational Physics (in Romanian and English)
- Numerical and Simulation Methods in Physics (in Romanian and English).

Administrative experience

- Head of the Dept. of Theoretical & Computational Physics, Babeş-Bolyai University (2000-11).
- Director of the Centre of International Cooperation, Babeş-Bolyai University (2008-11).

28.05.2020