UNIVERSITY BABEŞ-BOLYAI
FACULTY OF PHYSICS

LIST OF PUBLICATIONS

Prof. Dr. Titus Adrian Beu

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, 2014) 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.
   ISBN 978-3-527-31455-3

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.
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4. **T. A. Beu**,
   "Numerical Calculus in C, Third Edition",
   (MicroInformatica, Cluj-Napoca, 2004) 372 pp. (in Romanian).
   ISBN 973-9443-92-3

5. **T. A. Beu**,
   "Numerical Calculus in C, Second Edition",
   (MicroInformatica, Cluj-Napoca, 2000) 372 pp. (in Romanian).
   ISBN 973-9443-92-3

6. **T. A. Beu**,
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   Editors O.-G. Piringer and A.L. Baner (Wiley-VCH, Weinheim, New York, 2000) p. 221-238.
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   "Numerical Calculus in C",
   (MicroInformatica, Cluj-Napoca, 1999) 372 pp. (in Romanian).
   ISBN 973-9443-33-8

8. **T. A. Beu**,
   "Numerical Analysis in Turbo Pascal",
   (MicroInformatica, Cluj-Napoca, 1992) 204 pp. (in Romanian).
   ISBN 973-95718-5-9

Papers in refereed journals

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, 349-361 (2020), 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, 316-323 (2019), 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, 94-98 (2019), 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, 2564–2575 (2018), DOI:10.1002/jcc.25637.

6. A. Farcaş, **T. A. Beu**,
"Complexation of DNA with Cationic Polymers",
Studia UBB Chemia, LXIII, 2, 165 (2018).

7. **T. A. Beu**; Farcas,
"Structure and Dynamics of Solvated Polyethylenimine Chains",
AIP Conference Proceedings 1916, 020001 (2017), DOI: 10.1063/1.5017421.

8. **T. A. Beu**, A. Farcas,
"CHARMM force field and molecular dynamics simulations of protonated polyethylenimine",
J. Comput. Chem. **38**, 2335–2348 (2017), DOI: 10.1002/jcc.24890.

9. T. A. Beu and A. Farcas,
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10. L. Horvath, **T. Beu**, M. Manghi, and J. Palmeri,
"The vapor-liquid interface potential of (multi)polar fluids and its influence on ion solvation"
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11. S. Höfinger, A. Acocella, S. C. Pop, T. Narumi, K. Yasuoka, **T. Beu**, and F. Zerbetto,
"GPU-Accelerated Computation of Electron Transfer",
Journal of Computational Chemistry **33**, 2351–2356 (2012).

12. S. C. Pop, **T. A. Beu**,"Vibrations of polythiophenes",
Computational and Theoretical Chemistry **995**, 66–74 (2012) (J. Mol. Struc.-THEOCHEM).

13. **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",
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"Molecular dynamics simulations of ion transport through carbon nanotubes. II. Structural effects of the nanotube radius, solute concentration, and applied electric fields",
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15. A. Jurjiu, A. Volta, and **T. Beu**,
"Relaxation dynamics of a polymer network modeled by a multihierarchical structure",
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16. **T. A. Beu**, A. Jurjiu,
"Radiation-induced fragmentation of fullerenes",
Phys. Rev. B **83**, 024103-7 (2011).

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"Simulation of the flow of aqueous solutions through carbon nanotubes",
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"Molecular dynamics simulations of ion transport through carbon nanotubes. I. Influence of geometry, ion specificity and many-body interactions",
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19. M. V. Diudea, A. E. Vizitiu, **T. Beu**, A. Bende, C. L. Nagy, D. Janežic,
"Circulene covered fullerenes",
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20. **T. A. Beu**, L. Horvath, I. Ghişoiu,
"Tight-binding molecular dynamics simulations of radiation-induced C_{60} fragmentation",
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21. **T. A. Beu**,
"Simulations of radiation induced fragmentation of C_{60} fullerenes",
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22. L. Horvath, **T. A. Beu**,
"Tight-binding molecular dynamics simulations of radiation-induced fragmentation of C_{60}",
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"Infrared spectroscopy of large ammonia clusters as a function of size",
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"First-principles calculations of the vibrational spectra of one-dimensional C_{60} polymers",
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25. **T. A. Beu**,
"Simulations of biological ion channels by molecular dynamics",
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"Electronic structure calculations of peanut-shaped C_{60} polymers",
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29. **T. A. Beu**,
"MD Simulation of a Biological Ion Channel",
Bulletin of the Discrete Variational Xα Society of Japan, Vol. **17**, No.1, 33-37 (2004).

30. **T. A. Beu**,
"MD Simulations of Biological Ion Channels in Intense Magnetic Fields",
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31. **T. A. Beu**, C. Steinbach, U. Buck,
"Model analysis of the fragmentation of large H_2O and NH_3 clusters based on MD simulations",
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33. **T. A. Beu**, C. Steinbach, U. Buck,
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"Structural and vibrational properties of C_{36} and its oligomers $(C_{36})_{M=2,3,4}$ by tight-binding molecular dynamics",
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"Vibrational spectra of ammonia clusters from n=13 to 18",
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37. **T. A. Beu**, J. Onoe, K. Takeuchi,
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"Evidence for Chiral Isomers in the Spectra of Small Size Selected Hydrazine Clusters",
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41. **T. A. Beu**, J. Onoe, K. Takeuchi,
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45. **T. A. Beu**, J. Onoe, K. Takeuchi,
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J. Chem. Phys. **103**, 6394-6413 (1995).

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"Structures and IR-spectra of small SF_6 clusters. I. Potential model and cluster structures",
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50. **T. A. Beu**,
"Perturbation approach for frequency shifts in IR spectra of molecular clusters",
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51. **T. A. Beu**,
"Analytical torsion *L*-tensor formulas for anharmonic force constant transformation",
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"Fourth order torsion *L*-tensor formulas for anharmonic force constant transformation",
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"Gas Transport through Metallized Polymer Membranes",
Mater. Chem. Phys. **26**, 309-322 (1990).

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"Theoretical Approach to Gas Transport through Metallized Polymer Membranes",
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"Magnetohydrodynamic instability of a composite plasma in the presence of Rayleigh-Bénard effect. Dispersion equation",
Sci. Annals Univ. "Al.I. Cuza", series I.b. Physics, **35**, 61-67 (1989).

56. **T. A. Beu**, M.Vasiu,
"Transport in Tokamak Plasmas",
Studia Physica **34** (2), 94-100 (1989).

57. M. Vasiu, **T. A. Beu**,
"L'équation de dispersion d'un fluide visqueux élastique ionisé, en présence de l'effet Rayleigh-Bennard",
Studia Physica **33** (2), 53-57 (1988).

58. **T. A. Beu**, M. Vasiu,
"Rotational Excitation of NH_3 in Collisions with He",
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59. **T. A. Beu**, D. Simionovici, V. Anghel,
"GRENADE - a Coarse-mesh Reactor Physics Program to Solve the Static Diffusion Equation for Neutrons",
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60. **T. A. Beu**, M. Vasiu,
"Impurities Distributions in Tokamak Plasmas",
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"TOPIC - a Tokamak Plasma Impurities Code",
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62. **T. A. Beu**, D. Ciobotaru,
"Contours of Electron Beams from Shielded and Immersed Guns",
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"Prolate Radial Spheroidal Wave Functions",
Comput. Phys. Commun. **30**, 177-185 (1983).

64. **T. A. Beu**, R.I. Campeanu,
"Prolate Angular Spheroidal Wave Functions",
Comput. Phys. Commun. **30**, 187-192 (1983).

65. R.I. Campeanu, **T. A. Beu**,
"Hydrogen-Antihydrogen Interaction Potential",
Physics Letters **93A**, 223-226 (1983).

International Conferences (oral presentations 2017-2019)

1. **T. A. Beu**, A. Farcaş,
"CHARMM force field and molecular dynamics simulations of polyethylenimine chains",
4th International Conference on Physical and Theoretical Chemistry, (18-19 September 2017, Dublin, Ireland).
2. **T. A. Beu**, A. Farcaş, A. E. Ailenei,
"Atomistic and Coarse-Grained Modelling of Gene Delivery Polymers",
12th Joint Conference on Mathematics and Computer Science (12th MaCS), (14-17 June 2018, Săcuieu, Romania).
3. **T. A. Beu**, A. Farcaş, A. E. Ailenei,
"Atomistic and Coarse-Grained Modelling of Polyethylenimine for Gene Delivery Applications", Polymer World Congress 2018 (PWC 2018), (3–6 September 2018, Stockholm, Sweden).
(invited presentation)

4. **T. A. Beu**, A. Farcaş, A. E. Ailenei,
   "Coarse-grained modeling of polyethyleneimine",
   Molecular Modeling in Chemistry and Biochemistry Conference 2018 (MolMod 2018), (28-30 October 2018, Cluj-Napoca, Romania).
5. **T. A. Beu**, R. I. Costinaș, A. E. Ailenei,
   "Coarse-grained modeling of DNA-genetic-vector complexes",
   TIM19 Physics Conference, (29-31 May 2019, Timișoara, Romania).
   (plenary lecture)
6. **T. A. Beu**,
   "DNA-polycation complexes: coarse-grained modeling and simulations",
   2nd Euro Chemistry Conference, (17-19 June 2019, Valencia, Spain).
   (keynote speech)
7. **T. A. Beu**,
   "Coarse-grained simulations of DNA-polyethyleneimine complex formation",
   12th European Conference on Computational and Theoretical Chemistry (EUCO-CTC), (1-5 September 2019, Perugia, Italy).
8. **T. A. Beu**,
   "DNA-Polyethyleneimine complex formation: coarse-grain simulations",
   12th International Conference on Processes in Isotopes and Molecules (PIM19), (25-27 September 2019, Cluj-Napoca, Romania).

Papers in refereed conference proceedings

1. **Beu, Titus A**.; Farcas, Alexandra
   Tight-Binding Vibrational Analysis of Single-Wall Carbon Nanotubes
   Edited by: Vizman, D; Popescu, A
   Conference: TIM Physics Conference on Physics without Frontiers Location: W Univ Timisoara, Timisoara, ROMANIA Date: NOV 20-22, 2014
   Sponsor(s): Cent European Initiat
   TIM14 PHYSICS CONFERENCE: PHYSICS WITHOUT FRONTIERS Book Series: AIP Conference Proceedings
   Volume: 1694 Article Number: UNSP 020001 Published: 2015
2. **T. A. Beu**,
   Nanofluidic Transport and field-effect conductance in voltage-controlled carbon nanotubes,
   24th IUPAP Conference on Computational Physics (IUPAP-CCP 2012), Oct. 14-18, 2012, Kobe, Japan.
3. **T. A. Beu**,
   Molecular Dynamics simulations of ionic transport through voltage-controlled carbon nanotubes,
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   12th IEEE Conference on Nanotechnology (IEEE-NANO) 2012
   DOI: 10.1109/NANO.2012.6322070
   Publication Year: 2012 , Page(s): 1 – 5.
4. **T. A. Beu**,
   "Molecular dynamics simulations of fullerenes: from nanofluidics in carbon nanotubes to fragmentation of buckyballs",
   CCP2011 – Conference on Computational Physics, Gatlinburg, Tennessee, Oct. 23 – Nov. 4, 2011.
5. **T. A. Beu**,
   "Simulation of the flow of aqueous solutions through carbon nanotubes",
   CCP2010 – Conference on Computational Physics, Trondheim, Norway, June 23-26, 2010, pp. 188.
6. **T. A. Beu**,
   "Simulations of radiation induced fragmentation of C_{60} fullerenes",
   Modeling and Simulation of New Materials, Proceedings of Modeling and Simulation of New Materials: Tenth Granada Lectures, Granada, Spain, 15-19 September 2008, Series: AIP Conference Proceedings , Vol. 1091, Editors: Pedro L Garrido,. Pablo I. Hurtado, and Joaquín Marro, ISBN: 978-0-7354-0624-7, 2009, pp. 249-252.
7. **T. A. Beu**,
   "Efficient electrolyte modeling in MD simulations of bulk liquids, interfaces and ion channels",
   CCP2007, Conference on Computational Physics, Brussels, 5-8 September 2007, Université Libre de Bruxelles, Editor Michel Mareschal, pp. 325.

8. **T. A. Beu**,
   "MD simulations of bulk liquids, interfaces and ion channels",
   MOLMOD 2007, Molecular Modeling in Chemistry and Biochemistry, Cluj-Napoca, Romania, 5-8 July 2007.

9. **T. A. Beu**,
   "Efficient electrolyte modeling in MD simulations of transport in membrane channels",
   XX Sitges Conference, Physical Biology: from Molecular Interactions to Cellular Behavior, 5-9 June 2006, Sitges, Barcelona, Spain, pp. 90-91.

10. **T. A. Beu**,
    "Calculations of Structure and IR Frequency Shifts for Water and Ammonia Clusters",
    7th International Balkan Workshop on Applied Physics, July 5-7, 2006, Constanta, Romania (invited talk).

11. A.-M. Florescu, **T. A. Beu**,
    "Vibrational Frequency Shifts for (H2O)N Clusters, N ≤ 20",
    7th International Balkan Workshop on Applied Physics, July 5-7, 2006, Constanta, Romania.

12. L. Horvath, **T. A. Beu**,
    "Tight-Binding Molecular Dynamics Simulations of Radiation and Collision Induced Fragmentation of C_{60}",
    7th International Balkan Workshop on Applied Physics, July 5-7, 2006, Constanta, Romania.

13. **T. A. Beu**,
    "Simulation of the Ion Transport through Biological Membrane Channels",
    "Physics Conference TIM-05", West University of Timişoara, 25-26 November 2005.

14. **T. A. Beu**,
    "Simulations of Biological Ion Channels",
    Several Aspects of Biology, Chemistry, Informatics, Mathematics, and Physics – International Conference, University of Oradea, 11-13 November 2005.

15. **T. A. Beu**,
    MD Simulations of Biological Ion Channels,
    6th International Balkan Workshop on Applied Physics,
    July 5-7, 2005, Constanta, Romania.

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    "MD Simulations of Biological Ion Channels",
    6th International Balkan Workshop on Applied Physics,
    July 5-7, 2005, Constanta, Romania.

17. **T. A. Beu**,
    "MD Simulation of a Biological Ion Channel",
    "17th Discrete Variational Xα Conference",
    August 4-6, 2004, Kwansei University, Sengari, Japan.

18. **T. A. Beu**,
    "MD Simulations of Biological Ion Channels in Intense Magnetic Fields",
    "Advanced Spectroscopies on Biomedical and Nanostructured Systems",
    September 19-22, 2004, Cluj-Napoca, Romania.

19. **T. A. Beu**, C. Steinbach, U. Buck,
    "Intermolecular vibrations of large ammonia clusters from helium atom scattering",
    "The National Romanian Conference Of Theoretical Physics", 13-16 September 2002, Magurele, Bucharest, Romania.

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    "Theoretical study of the structure and IR frequency shift for small SF6 and UF6 clusters",
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    "Structure and IR-spectrum calculations for small SF6 and UF6 clusters",
    "Gordon Research Conference on Molecular and Ionic Clusters", Il Ciocco, Tuscany, Italy, 5-10 May, 1996.

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    "Structure and IR-spectrum calculations for small clusters of XY6-type molecules",
    "1995 Fall Meeting of the Atomic Energy Society of Japan", Tokai, 17-20 Oct. 1995, pp. 530.

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"Proceedings of the 6th Joint EPS-APS International Conference on Physics Computing - Physics Computing '94", Lugano, Switzerland, 22-26 August 1994, Editors: R. Gruber and M. Tomasini, European Physical Society, pp. 313-316.

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"Rotational Molecular Scattering Calculations",
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27. **T. A. Beu**,
"Micro-TOPIC: A Tokamak Plasma Impurities Code",
"Proceedings of the 4th International Conference - Physics Computing '92", Prague, Czechoslovakia, August 24-28, 1992, Editors: R.A. de Groot and J. Nadrchal, World Scientific, pp. 266-267.

28. **T. A. Beu**, G. Damian,
"NH_3-He and NH_3-H_2 Rotational Scattering Calculations",
"XXI. European Congress on Molecular Spectroscopy, EUCMOS XXI", August 23-28, 1992 Vienna, Austria.

29. **T. A. Beu**,
"Studies Concerning Impurities Transport Anomality in Tokamak Plasmas",
"1st Congress of the Balkan Physical Union", September 26-28, 1991, Thessaloniki, Greece, pp. 2-05.

Textbooks and curriculum material

1. **T. A. Beu**,
"Quantenmechanik I",
(University "Babeş-Bolyai" Press, Cluj-Napoca, 2000) 134 p. (in German)
http://www.phys.ubbcluj.ro/~titus.beu/teaching.html (electronic lecture notes)

2. **T. A. Beu**,
"Molecular Dynamics Simulations" (electronic lecture notes)
http://www.phys.ubbcluj.ro/~titus.beu/teaching.html.

3. **T. A. Beu**,
"Numerical Methods for Physicists" (electronic lecture notes)
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