UNIVERSITATEA “BABEŞ-BOLYAI” CLUJ-NAPOCA
FACULTATEA DE FIZICĂ

LISTA PUBLICAŢIILOR ŞTIINŢIFICE

Prof. Dr. Titus Adrian Beu

Monografii în edituri consacrate din străinătate

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.
   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.
   doi: 10.1002/9783527613281.ch08, ISBN 978-3-527-28868-7

4. **T. A. Beu**,
   “Numerical solutions of the diffusion equation”, in *Plastic Packaging Materials for Food*,
   Editors O.-G. Piringer and A.L. Baner (Wiley-VCH, Weinheim, New York, 2000) p. 221-238.
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1. **T. A. Beu**,
   “Calcul numeric în C”, Ediţia a III-a,
   (Editura Albastră, MicroInformatica, Cluj-Napoca, 2004) 372 p.
   ISBN 973-9443-92-3

2. **T. A. Beu**,
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   ISBN 973-9443-92-3

3. **T. A. Beu**,
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4. **T. A. Beu**,
   “Analiză numerică în Turbo Pascal”,
   (MicroInformatica, Cluj-Napoca, 1992) 204 p.
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1. **T. A. Beu**, A. Bende, A.-A. Farcaș,
   “Calculations of electron transfer in the tris[4-(2-thienyl)phenyl]amine–C70 donor-acceptor system”,
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2. **T. A. Beu**, A. E. Ailenei, R. I. Costinaș,
   “Martini Force Field for Protonated Polyethyleneimine”,
   J. Comput. Chem. 41, 349-361 (2020), DOI: 10.1002/jcc.26110.

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"Light-induced spin transitions in Ni(II)-based macrocyclic-ligand complexes: A DFT study",
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"Atomistic and Coarse-Grained Modeling of Polyethyleneimine",
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"CHARMM Force Field for Protonated Polyethyleneimine",
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6. A. Farcaş, **T. A. Beu**,
"Complexation of DNA with Cationic Polymers",
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9. T. A. Beu and A. Farcas,
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"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",
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12. S. C. Pop, **T. A. Beu**,"Vibrations of polythiophenes",
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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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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",
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17. **T. A. Beu**,
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19. M. V. Diudea, A. E. Vizitiu **T. Beu**, A. Bende, C. L. Nagy, D. Janezˇic,
"Circulene covered fullerenes",
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"Tight-binding molecular dynamics simulations of radiation-induced C_{60} fragmentation",
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"Model analysis of the fragmentation of large H_2O and NH_3 clusters based on MD simulations",
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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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"Calculations of structures and vibrational spectra of homogeneous and mixed SF_6 clusters with Ar",
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"Calculations of structures and vibrational spectra of acetonitrile clusters",
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"Analytical torsion *L*-tensor formulas for anharmonic force constant transformation",
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48. **T. A. Beu**, F. Spineanu, M. Vlad, R.I. Campeanu, I.I. Popescu,
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"Prolate Angular Spheroidal Wave Functions",
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"Hydrogen-Antihydrogen Interaction Potential",
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1. Tight-Binding Vibrational Analysis of Single-Wall Carbon Nanotubes
   By: Beu, Titus A.; Farcas, Alexandra
   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**,
   "Molecular Dynamics Simulations of Ionic Transport through Voltage-Controlled Carbon Nanotubes",
   IEEE NANO 2012 - 12th International Conference on Nanotechnology
   20 - 23 August 2012, Birmingham, UK (DOI: 10.1109/NANO.2012.6322070, IEEE Xplore online)

3. **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",
   Virtual Journal of Nanoscale Science & Technology - August 15, Volume 24, Issue 7 (2011),
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   "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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6. **T. A. Beu**, L. Horvath, I. Ghisoiu,
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"Limitele cunoașterii în lumea cuantelor",
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"Theoretical Approach to Gas Transport through Metallized Polymer Membranes",
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Conferințe internaționale (prezentări orale 2017-2019)

15. **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).
16. **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).
17. **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)
18. **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).
19. **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)
20. **T. A. Beu**,
"DNA-polycation complexes: coarse-grained modeling and simulations",
2nd Euro Chemistry Conference, (17-19 June 2019, Valencia, Spain).
(keynote speech)
21. **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).
22. **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).

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1. **Beu, Titus A**.; Farcas, Alexandra,
Tight-Binding Vibrational Analysis of Single-Wall Carbon Nanotubes,
TIM14 Physics Conference: Physics without Frontiers W Univ Timisoara, Nov. 20-22, 2014, AIP Conference Proceedings, Volume: 1694, Article Number: UNSP 020001.

2. **T. A. Beu**,
Nanofluidic Transport and field-effect conductance in voltagecontrolled carbon nanotubes,
24th IUPAP Conference on Computational Physics (IUPAP-CCP 2012), Oct. 14-18, 2012, Kobe, Japan.

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Conference on Computational Physics CCP2012, 14-18 Oct. 2012, Kobe, Japan
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5. **T. A. Beu**,
„Molecular dynamics simulations of fullerenes: from nanofluidics in carbon nanotubes to fragmentation of buckyballs",
The 3rd Workshop on Computational and Statistical Physics (CSP3), Kyoto, Japan, 19-20 Oct. 2012
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6. **Beu, Titus Adrian**,
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9. **T. A. Beu**,
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   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.

10. **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.

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    MOLMOD 2007, Molecular Modeling in Chemistry and Biochemistry, Cluj-Napoca, Romania, 5-8 July 2007.

12. **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).

13. A.-M. Florescu, **T. A. Beu**,
    “Vibrational Frequency Shifts for $(H2O)_N$ Clusters, $N \leq 20$”,
    7th International Balkan Workshop on Applied Physics, July 5-7, 2006, Constanta, Romania.

14. 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.

15. **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.

16. **T. A. Beu**,
    “Simulation of the Ion Transport through Biological Membrane Channels”,
    “Physics Conference TIM-05”, West University of Timişoara, 25-26 November 2005 (invited talk).

17. **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 (invited talk).

18. **T. A. Beu**,
    ”Electronic Structure Calculations of Peanut-Shaped C_{60} Polymers”,
    6th International Balkan Workshop on Applied Physics, July 5-7, 2005, Constanta, Romania (invited talk).

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    ”MD Simulations of Biological Ion Channels”,
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    ”MD Simulations of Biological Ion Channels in Intense Magnetic Fields”,
    Advanced Spectroscopies on Biomedical and Nanostructured Systems, September 19-22, 2004, Cluj-Napoca, Romania.

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    ”MD Simulation of a Biological Ion Channel”,
    17th Discrete Variational Xα Conference, August 4-6, 2004, Kwansei University, Sengari, Japan (invited talk).

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    “Theoretical study of the structure and IR frequency shift for small SF_6 and UF_6 clusters”,
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