

## Publication Lists (2001 – present):



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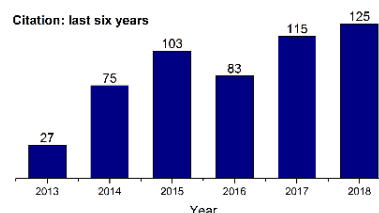
**Total number of publications: 87**

**Total number of ISI publications: 68**

**Total number of independent ISI citations: 646**

**Hirsch index: 11**

[Publons](#), [Scopus](#), [Google Scholar](#) or [Publication List](#).



### Articles (ISI)

1. C. Sacalis, C. Morar, P. Lameiras, A. Lupan, R. Silaghi-Dumitrescu, **A. Bende**, G. Katona, D. Porumb, D. Harakat, E. Gál, M. Darabantu: „*Design, synthesis and structure of novel dendritic G-2 melamines comprising piperidine motifs as key linkers and 4-(n-octyloxy)aniline as a peripheral unit*”, *Tetrahedron*, **75**(35), 130468 (2019). ([PDF](#))
2. L. Almásy, **A. Bende**: „*Intermolecular interaction in methylene halide (CH<sub>2</sub>F<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>, CH<sub>2</sub>Br<sub>2</sub> and CH<sub>2</sub>I<sub>2</sub>) dimers*”, *Molecules*, **24**(9), 1810 (2019). ([PDF](#))
3. A.-A. Farcaș, T. A. Beu, **A. Bende**: „*Light-induced spin transitions in Ni(II)-based macrocyclic-ligand complexes: A DFT study*”, *Journal of Photochemistry and Photobiology A: Chemistry*, **376**, 316-323 (2019). ([PDF](#))
4. G. Borodi, A. Turza, O. Onija, A. Bende: “*Succinic, fumaric, adipic and oxalic acid cocrystals of promethazine hydrochloride*”, *Acta Crystallographica C*, **C75**, 107–119 (2019). ([PDF](#))
5. A. Bende, M. F. Gaele, T. M. Di Palma: “*UV Photoionization of Sodium-Doped Formic Acid Clusters*”, *CHEMPHYSICHEM*, **19**(20), 2724–2734 (2018). ([PDF](#))
6. C. Morar, P. Lameiras, A. Bende, G. Katona, E. Gál, M. Darabantu: “*Design, synthesis and structure of novel G-2 melamine-based dendrimers incorporating 4-(n-octyloxy)aniline as a peripheral unit*”, *Beilstein Journal of Organic Chemistry*, **14**, 1704–1722 (2018). ([PDF](#))
7. C. Lar, A. Woiczehowski-Pop, **A. Bende**, I. G. Grosu, N. Miklášová, E. Bogdan, N. D. Hădade, A. Terec, I. Grosu: „*A three-armed cryptand with triazine and pyridine units: synthesis, structure and complexation with polycyclic aromatic compounds*”, *Beilstein Journal of Organic Chemistry*, **14**, 1370–1377 (2018). ([PDF](#))
8. A. Petran, N. D. Hădade, C. Filip, X. Filip, **A. Bende**, A. Popa, J. Liebscher: “*Poly[3,4-dihydroxybenzhydrazide]: A Polydopamine Analogue?*”, *Macromolecular Chemistry and Physics*, **219**(10), 1700564 (2018). ([PDF](#))
9. M. Coroș, F. Pogăcean, L. Măgerușan, M.-C. Roșu, A. S. Porav, C. Socaci, **A. Bende**, R.-I. Stefan-van Staden, S. Pruneanu: “*Graphene-porphyrin composite synthesis through graphite exfoliation: The electrochemical sensing of catechol*”, *Sensors and Actuators B: Chemical*, **256**, 665 – 673 (2018). ([PDF](#))
10. A. Bende: “*Low-Lying Excited States and Their Relaxation Pathways of Phenothiazine*”, *AIP Conference Proceedings*, **1917**, 020002 (2017). ([PDF](#))
11. I. G. Grosu, M. I. Rednic, M. Miclăuș, I. Grosu, **A. Bende**: “*The nature of intermolecular interactions in pyridinium–anion–β-hexachlorocyclohexane molecular crystals*”, *Physical Chemistry Chemical Physics*, **19**(31), 20691 – 20698 (2017). ([PDF](#))
12. C. Morar, G. L. Turdean, **A. Bende**, P. Lameiras, C. Antheaume, L. M. Muresan, M. Darabantu: “*New p-aminophenol-based dendritic melamines. Iterative synthesis, structure, and electrochemical characterisation*”, *Comptes Rendus Chimie*, **20**, 402 – 414 (2017). ([PDF](#))
13. A. R. Deac, C. Morar, G. L. Turdean, M. Darabantu, E. Gál, **A. Bende**, L. M. Muresan: “*Glassy carbon electrode modified with hemin and new melamine compounds for H<sub>2</sub>O<sub>2</sub> amperometric detection*”, *Journal of Solid State Electrochemistry*, **20**(11), 3071 – 3081 (2016). ([PDF](#))
14. H. Popeneciu, D. Ristoiu, I. Bratu, G. Borodi, A. Bende, L. Barbu: “*Inclusion compounds of β-cyclodextrin-pitofenone hydrochloride. Investigations of solid forms*”, *Studia UBB Chemia*, **61**(2), 61 – 71 (2016).
15. M. I. Rednic, R. A. Varga, **A. Bende**, I. G. Grosu, M. Miclăuș, N. D. Hădade, A. Terec, E. Bogdan, I. Grosu: “*Supramolecular anion recognition by β-HCH*”, *Chemical Communications*, **52**, 12322 – 12325 (2016). ([PDF](#))

16. **A. Bende**, G. Perretta, P. Sementa, T. M. Di Palma: "Inception of acetic acid-water cluster growth in molecular beams", *CHEMPHYSICHEM*, **16**(14), 3021 – 3029 (2015). ([PDF](#))
17. T. M. Di Palma and **A. Bende**: "Encasing of Na<sup>+</sup> ion in dimer-formed acetic acid clusters", *Journal of Mass Spectrometry*, **50**(10), 1136 – 1143 (2015). ([PDF](#))
18. M. Vlassa and **A. Bende**: "Theoretical investigation of polymer chain stability in the metal coordinated azorubine and cyclam complex", *Chemical Physics*, **457**, 152–159 (2015). ([PDF](#))
19. **A. Bende**, V. Toşa: "Modeling laser induced molecule excitation using real-time time-dependent density functional theory: Application to 5- and 6-benzyluracil", *Physical Chemistry Chemical Physics*, **17**(8), 5861 – 5871 (2015). ([PDF](#))
20. A. Woiczehowski-Pop, D. Gligor, **A. Bende**, C. Varodi, E. Bogdan, A. Terec, I. Grosu: "Synthesis, structure, electrochemical behaviour and electrochemical investigations on the assembling with pyrene of a novel C<sub>3</sub> cryptand", *Supramolecular Chemistry*, **27**(1-2), 52 – 58 (2015). ([PDF](#))
21. A. Csehi, **A. Bende**, G. J. Halász, Á. Vibók, A. Das, D. Mukhopadhyay, S. Mukherjee, S. Adhikarie, M. Baer: "Dressed Adiabatic and Diabatic Potentials to study Topological Effects for F + H<sub>2</sub> System", *Journal of Physical Chemistry A*, **118**(33), 6361 – 6366 (2014). ([PDF](#))
22. J. Ladik, **A. Bende**: "Quantum Molecular Biological Investigation of the Onset of Cancer", *International Journal of Quantum Chemistry*, **114**(18), 1229 – 1235 (2014). ([PDF](#))
23. T. M. Di Palma, **A. Bende**: "Tautomerism and proton transfer in photoionized acetaldehyde and acetaldehyde-water clusters", *Journal of Mass Spectrometry*, **49**(8), 700 – 708 (2014). ([PDF](#))
24. F. Bogár, **A. Bende**, J. Ladik: "Influence of the sequence on the ab initio band structures of single and double stranded DNA models", *Physics Letters A*, **378**, 2157 – 2162 (2014). ([PDF](#))
25. **A. Bende**, C. M. Muntean: "The influence of anharmonic and solvent effects on the theoretical vibrational spectra of the guanine–cytosine base pairs in in Watson–Crick and Hoogsteen configurations", *Journal of Molecular Modeling*, **20**(3), Article No: 2113, (2014). ([PDF](#))
26. M. V. Diudea, Cs. L. Nagy, **A. Bende**: "Carbon multi-shell cages", *Physical Chemistry Chemical Physics*, **16**(11), 5260 - 5269 (2014). ([PDF](#))
27. **A. Bende**: "Low-lying excited-states and relaxation pathways of acetophenone", *AIP Conf. Proc.*, **1565**, 24 - 28 (2013). ([PDF](#))
28. A. Csehi, **A. Bende**, G. J. Halász, A. Vibók, A. Das, D. Mukhopadhyay, S. Mukherjee, S. Adhikarie, and M. Baer: "Dressed Adiabatic and Diabatic Potentials for the Renner-Teller/Jahn-Teller F+H<sub>2</sub> System", *Journal of Physical Chemistry A*, **117**(36) 8497–8505 (2013). ([PDF](#))
29. J. Liebscher, R. Mrówczyński, H. A. Scheidt, C. Filip, N. D. Hädade, R. Turcu, **A. Bende**, S. Beck: "The Structure of Polydopamine – a Never Ending Story?", *Langmuir*, **29**(33), 10539–10548 (2013). ([PDF](#))
30. M. Micciarelli, C. Altucci, B. Della Ventura, R. Velotta, V. Toşa, A. B. González Pérez, M. Pérez Rodríguez, Á. R. de Lera, **A. Bende**: "Low-lying excited-states of 5-benzyluracil", *Physical Chemistry Chemical Physics*, **15**, 7161 - 7173 (2013). ([PDF](#))
31. **A. Bende**, F. Bogár, J. Ladik: "Hole mobilities of periodic models of DNA double helices in the nucleosomes at different temperatures", *Chemical Physics Letters*, **565**, 128 - 131 (2013). ([PDF](#))
32. T. M. Di Palma, **A. Bende**: "Vacuum Ultraviolet Photoionization and ab initio Investigations of Methyl Tert-Butyl Ether (MTBE) Clusters and MTBE – Water Clusters", *Chemical Physics Letters*, **561-562**, 18 - 23 (2013). ([PDF](#))
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34. V. Boldescu, I. Bratu, Gh. Borodi, I. Kacsó, **A. Bende**, Gh. Duca, F. Macaev, S. Pogrebnoi, Z. Ribkovskaia: "Study of binary systems of β-cyclodextrin with a highly potential anti-mycobacterial drug", *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **74**, 129 – 135 (2012). ([PDF](#))
35. O. Bradea, I. Kacsó, Gh. Borodi, **A. Bende**, I. Bratu: "Complexation of Amlodipine Besylate with β-Cyclodextrin", *Acta Chimica Slovenica*, **59**, 18 – 23, (2012). ([PDF](#))
36. M. V. Diudea, Cs. L. Nagy, **A. Bende**: "On Diamond D5", *Structural Chemistry*, **23**(4), 981 – 986 (2012). ([PDF](#))
37. **A. Bende**, C. M. Muntean: "Solvent effect on the anharmonic vibrational frequencies in guanine-cytosine base pair", *AIP Conf. Proc.*, **1425**, 5 - 8 (2012). ([PDF](#))

38. S. Dreve, I. Kacsó, A. Popa, O. Raita, **A. Bende**, Gh. Borodi, I. Bratu: "Chitosan-Based Nanocarriers For Antimalarials", AIP Conf. Proc., **1425**, 17 - 21 (2012). ([PDF](#))
39. **A. Bende**, F. Bogár, J. Ladik: "Possible role of  $Cl^-$  ions in DNA-protein interactions in the nucleosomes", Chemical Physics Letters, **525 – 526**, 115 – 119 (2012). ([PDF](#))
40. **A. Bende**, D. Bogdan, C. M. Muntean, C. Morari: "Localization and anharmonicity of the vibrational modes for the GC Watson-Crick and Hoogsteen base pairs", Journal of Molecular Modeling, **17**(12), 3265 - 3274 (2011). ([PDF](#))
41. **A. Bende**, L. Almásy: "Weakly bonded cluster structures of *N,N'*-dimethylethyleneurea and water" Journal of Molecular Liquids, **162**, 45 – 49 (2011). ([PDF](#))
42. S. Dreve, I. Kacsó, A. Popa, O. Raita, F. Dragan, **A. Bende**, Gh. Borodi, I. Bratu: "Structural Investigation of Chitosan-based Microspheres with some Anti Inflammatory Drugs", Journal of Molecular Structure, **997**(1-3), 78-86 (2011). ([PDF](#))
43. **A. Bende**, I. Turcu: "Nitrogen Substituted Phenothiazine Derivatives: Modeling of Molecular Self-Assembling", International Journal of Molecular Sciences (Special Issue "Advances in Molecular Electronic Structure Calculations"), **12**(5), 3102-3116, (2011). ([PDF](#))
44. **A. Bende**, F. Bogár, J. Ladik: "Model calculations of the energy band structures of double stranded DNA in the presence of water and  $Na^+$  ions", Solid State Communications, **151**(4), 301 - 305 (2011). ([PDF](#))
45. L. Almásy, **A. Bende**: "Ab initio structures of interacting methylene chloride molecules with comparison to the liquid phase", Journal of Molecular Liquids, **158**(3), 205 - 207 (2011). ([PDF](#))
46. **A. Bende**, I. Grosu, I. Turcu: "Molecular Modeling of Phenothiazine Derivatives: Self-Assembling Properties", Journal of Physical Chemistry A, **114**(47) 12479 – 12489 (2010). ([PDF](#))
47. T. M. Di Palma, **A. Bende** and A. Borghese: "Photoionisation and Structures of Jet-Formed Toluene Clusters", Chemical Physics Letters, **495**(1-3), 017 – 023 (2010). ([PDF](#))
48. M. V. Diudea, **A. Bende**, D. Janežič: "Omega polynomial in diamond-like networks", Fullerenes, Nanotubes and Carbon Nanostructures, **18**(3), 236 – 243 (2010). ([PDF](#))
49. **A. Bende**, F. Bogár, F. Beleznyay, J. Ladik: "Model calculation of the specific hole conductivities of the three homopolynucleotides, poly(guanilic acid), poly(adenilic acid) and polythymidine in presence of water and  $Na^+$  ions", Solid State Communications, **150**(9-10), 446 – 449 (2010). ([PDF](#))
50. **A. Bende**: "Hydrogen bonding in urea dimers and adenine-thymine DNA base pair: Anharmonic effects in intermolecular H-bond and intramolecular H-stretching vibrations", Theoretical Chemistry Accounts, **125**(3-6), 253 – 268 (2010). ([PDF](#))
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52. **A. Bende**, I. Turcu: "Molecular modeling of the weakly bounded dimers of some phenothiazine derivatives", Journal of Physics: Conference Series, **182**, 012001 (2009). ([PDF](#))
53. M. V. Diudea, A. E. Vizitiu, T. A. Beu, **A. Bende**, Cs. L. Nagy and D. Janežič: "Circulene covered fullerenes", Journal of Molecular Structure: THEOCHEM, **904**, 28 – 34 (2009). ([PDF](#))
54. N. Toşa, **A. Bende**, R. A. Varga, A. Terec, I. Bratu, I. Grosu: "H-bond-Driven Supramolecular Architectures of the Syn and Anti Isomers of the Dioxime of Bicyclo[3.3.1]nonane-3,7-dione", Journal of Organic Chemistry, **74**(10), 3944 – 3947 (2009). ([PDF](#))
55. **A. Bende**, F. Bogár, J. Ladik: "A Simple Model for the Band Structure and D.C. Conductivity of an Infinite  $C=O \cdots H-N$  Chain Perpendicular to the Protein Backbone", International Journal of Quantum Chemistry, **109**(3), 612 – 617 (2009). ([PDF](#))
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62. **A. Bende**, S. Suhai: "BSSE-corrected geometry, harmonic and anharmonic vibrational frequencies of formamide-water and formamid-formamide dimers", *International Journal of Quantum Chemistry*, **103**(6), 841-853 (2005). ([PDF](#))
63. **A. Bende**, Á. Vibók, G. J. Halász, S. Suhai: "Theoretical Study of Hydrogen Bonds between Acetylene and Selected Proton Donor Systems", *International Journal of Quantum Chemistry*, **101**(2), 186-200 (2005). ([PDF](#))
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66. **A. Bende**, Á. Vibók, G. J. Halász, S. Suhai: "BSSE-free Description of the Formamide Dimers", *International Journal of Quantum Chemistry*, **84**, 617-622 (2001). ([PDF](#))

#### **Book or Book Chapters:**

1. **A. Bende** (2015) *Modeling Laser-Induced Molecule Excitations Using Real-Time, Time-Dependent Density Functional Theory* In: Annual Reports in Computational Chemistry, Edited by: D. A. Dixon, Vol. 11, Page: 103 – 146, Elsevier Science, ISBN: 978-0-444-63710-9 ([WEB](#))
2. M. V. Diudea, B. Szeffler, Cs. L. Nagy, **A. Bende** (2015) *Exotic allotropes of carbon* In: Exotic Properties of Carbon Nanomatter, Edited by: M. V. Putz, O. Ori, Book Series: Carbon Materials: Chemistry and Physics, Vol. 8, Page: 185 – 201 Springer: Dordrecht, The Netherlands, ISBN: 978-94-017-9566-8 ([WEB](#))
3. **A. Bende**, M. V. Diudea (2013) *Energetics of multi-shell cages* In: Diamond and Related Nanostructures, Edited by: M. V. Diudea and Cs. L. Nagy, Book Series: Carbon Materials: Chemistry and Physics, Vol. 6, Page: 107 – 120, Springer, ISBN-13: 978-94-007-6370-8. ([WEB](#))
4. A. E. Vizitiu, M. V. Diudea, T. A. Beu, **A. Bende** (2011) *Fullerene aromaticity by circulene-flower coverings* In: Advances in Chemical Modeling Edited by: Mihai V. Putz, Page: 361 – 367, New York: Nova Science Publisher, Inc. ISBN: 978-1-61209-028-3. ([WEB](#))
5. **A. Bende** (2011) *Chapter 8: Anharmonic effects in normal mode vibrations: their role in biological systems* In: Quantum Frontiers of Atoms and Molecules, Edited by: Mihai V. Putz. Page: 157 – 190, New York: Nova Science Publisher, Inc. ISBN: 978-1-61668-158-6. ([WEB](#))

#### **Articles (non-ISI):**

1. **A. Bende**: "The role of different positively and negatively charged ions on the stability of the histone nucleosome core particle", *Studia UBB Biologia Special Issue*, **60**, 53 – 56 (2015).
2. **A. Bende**, V. Toşa: "The role of the internal rotation on the 5-benzyluracil excited states", *Tier 2 Federation Grid, Cloud & High Performance Computing Science (RO-LCG) Conference Proceedings*, 15 – 18 (2012).
3. **Bende**, L. Almásy: "Ab initio study of mixed clusters of water and N, N'-dimethylethyleneurea", *Ukrainian Journal of Physics*, **56**(8), 796 – 800 (2011).
4. F. Fărcaş, G. Popeneacu, **A. Bende**, C. Morari, S. Belov, L. Miclea: "ITIM distributed grid system applied in high energy, biomolecular and nanotechnology physics", 2008 IEEE International Conference on Automation, Quality and Testing, Robotics, AQTR 2008 - THETA 16th Edition - Proceedings **3**, 343–346 (2008).
5. A. E. Vizitiu, M. V. Diudea, T. A. Beu, **A. Bende**: "Fullerene Aromaticity by Circulene-Flower Coverings", *International Journal of Chemical Modeling*, **1**(1), 7 – 14 (2008).
6. A. Nan, I. Crăciunescu, **A. Bende**, R. Turcu, D. Reichert, J. Liebscher: "Synthesis and Structure Investigations of Functionalized Polypyrrole Copolymers", *Journal of Nanostructured Polymers and Nanocomposites*, **4**(1), 3 – 12 (2008).
7. V. V. Morariu, O. Zainea, **A. Bende**, O. Popescu: "The Statistical Physics of Microbial Genomes: Part I. Organisation of Coding Sequencies in the Chromosome of Escherichia Coli", *Romanian Journal of Biophysics*, **16**(2), 103 – 110 (2006).

8. **A. Bende**, S. Suhai: "*H-Bond Vibrations in Ammonia - Ammonia and Ammonia - Water Dimers*", Acta Physica et Chimica Debrecina, **38-39**, 55 – 69 (2005).
9. **A. Bende**, V. Toşa: "*IR Multiphoton Absorption Spectra of Some Freon Molecules Used in <sup>13</sup>C Isotope Separation*", Asian Journal of Physics, **15**(2), 275 – 281 (2005).
10. N. Toşa, **A. Bende**, I. Bratu, I. Grosu: "*Theoretical Modeling and Experimental Study of Intramolecular Hydrogen-bond in Tetramethyl 3,7 – dihydroxy-bicyclo-[3.3.1]-nona-2,6-diene-2,4,6,8-tetracarboxylate*", Studia UBB Chemia, **50**(2), 157 – 162 (2005).
11. V. Toşa, **A. Bende**, T. D. Silipas, H. T. Kim, C. H. Nam: "*Modelling Plasma Fluorescence Induced by Femtosecond Pulse Propagation in Ionizing Gases*", Romanian Journal of Physics, **50**(7-8), 741 – 748 (2005).
12. **A. Bende**, V. Toşa: "*Geometry Structure and IR Multiphoton Excitation Spectra of SiF<sub>2</sub>H<sub>2</sub>. A theoretical study*", Acta Physica et Chimica Debrecina, **37**, 51 – 68 (2004).
13. N. Toşa, **A. Bende**, S. Cântă-Pânzaru, I. Grosu, E. Surducan: "*Structure and Vibrational Spectra of Tetramethyl 3,7-dihydroxybicyclo[3.3.1]nona-2,6-diene- 2,4,6,8-tetracarboxylate and Bicyclo[3.3.1]-nonane-3,7-dione*", Studia UBB Physica, **44**(3), 289 – 292 (2004).
14. **A. Bende**, Á. Vibók, G. J. Halász, S. Suhai: "*Ab initio Study of the Ammonia - Water Dimer. BSSE-free Structures and Intermolecular Harmonic Vibrational Frequencies*", Acta Physica et Chimica Debrecina, **36**, 7 – 23 (2003).
15. **A. Bende**, V. Toşa: "*Ab Initio Density Functional Study of CF<sub>2</sub>HCl and its isotopic species*", STUDIA UBB Physica Special Issue, **48**(2), 453 – 456 (2003).
16. **A. Bende**, V. Toşa: "*A Model for Infrared Multiple Photon Excitation of CF<sub>2</sub>HCl*", Roumanian Reports in Physics, **51**, 917–922 (1999).
17. A. Hamza, **A. Bende**: "*(SF<sub>6</sub>)<sub>n</sub>- Ar<sub>m</sub> Cluster Structures*", STUDIA UBB Physica, **42**(2), 55 – 65 (1997).