# Atilla Bende

List of Publications by Year
in descending order

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| 88 | 1,467 | 623734 | 345221 |
|---|---|---|---|
| papers | citations | 14 h-index | 36 g-index |

| 88 | 88 | 88 | 2549 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Structure of Polydopamine: A Never-Ending Story?. Langmuir, 2013, 29, 10539-10548. | 3.5 | 834 |
| 2 | Graphene-porphyrin composite synthesis through graphite exfoliation: The electrochemical sensing of catechol. Sensors and Actuators B: Chemical, 2018, 256, 665-673. | 7.8 | 46 |
| 3 | BSSE-corrected geometry and harmonic and anharmonic vibrational frequencies of formamide-water and formamide-formamide dimers. International Journal of Quantum Chemistry, 2005, 103, 841-853. | 2.0 | 31 |
| 4 | Hydrogen bonding in the urea dimers and adenineâ€“thymine DNA base pair: anharmonic effects in the intermolecular H-bond and intramolecular H-stretching vibrations. Theoretical Chemistry Accounts, 2010, 125, 253-268. | 1.4 | 27 |
| 5 | The electronic structure of the four nucleotide bases in DNA, of their stacks, and of their homopolynucleotides in the absence and presence of water. Journal of Chemical Physics, 2008, 128, 105101. | 3.0 | 21 |
| 6 | Halogen Bonds (N---I) at Work: Supramolecular Catemeric Architectures of 2,7-Dipyridylfluorene with ortho-, meta-, or para-Diiodotetrafluorobenzene Isomers. Crystal Growth and Design, 2020, 20, 3429-3441. | 3.0 | 17 |
| 7 | Calculation of the band structure of polyguanilic acid in the presence of water and Na+ ions. Journal of Chemical Physics, 2007, 127, 055102. | 3.0 | 16 |
| 8 | Molecular Modeling of Phenothiazine Derivatives: Self-Assembling Properties. Journal of Physical Chemistry A, 2010, 114, 12479-12489. | 2.5 | 16 |
| 9 | A tri-atomic Renner-Teller system entangled with Jahn-Teller conical intersections. Journal of Chemical Physics, 2013, 138, 024113. | 3.0 | 16 |
| 10 | BSSE-free description of the formamide dimers. International Journal of Quantum Chemistry, 2001, 84, 617-622. | 2.0 | 15 |
| 11 | BSSE-free description of intermolecular force constants in hydrogen fluoride and water dimers. International Journal of Quantum Chemistry, 2003, 92, 152-159. | 2.0 | 14 |
| 12 | Photoionisation and structures of jet-formed toluene clusters. Chemical Physics Letters, 2010, 495, 17-23. | 2.6 | 14 |
| 13 | Diamond and Related Nanostructures. Carbon Materials, 2013, , . | 1.2 | 14 |
| 14 | Low-lying excited-states of 5-benzyluracil. Physical Chemistry Chemical Physics, 2013, 15, 7161. | 2.8 | 14 |
| 15 | Structural investigation of chitosan-based microspheres with some anti-inflammatory drugs. Journal of Molecular Structure, 2011, 997, 78-86. | 3.6 | 13 |
| 16 | Dressed Adiabatic and Diabatic Potentials To Study Topological Effects for F + H<sub>2</sub>. Journal of Physical Chemistry A, 2014, 118, 6361-6366. | 2.5 | 13 |
| 17 | Weak intermolecular bonding in N,Nâ€²-dimethylethyleneurea dimers and N,Nâ€²-dimethylethyleneureaâ€“water systems: The role of the dispersion effects in intermolecular interaction. Chemical Physics, 2008, 354, 202-210. | 1.9 | 12 |
| 18 | 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, 2009, 74, 3944-3947. | 3.2 | 12 |

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|---|---|---|---|
| 19 | On diamond D5. Structural Chemistry, 2012, 23, 981-986. | 2.0 | 12 |
| 20 | Sugar matters: sugar moieties as reactivity-tuning factors in quercetin O-glycosides. Food and Function, 2020, 11, 5293-5307. | 4.6 | 12 |
| 21 | Charge transfer between the <mml:math altimg="si3.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www... Chemical Physics | 2.6 | 11 |
| 22 | Halogen-Bonded Organic Frameworks of Perfluoroiodo- and Perfluorodiiodobenzene with 2,2â€²,7,7â€²-Tetrapyridyl-9,9â€²-spirobifluorene. Crystal Growth and Design, 2021, 21, 1045-1054. | 3.0 | 11 |
| 23 | Model calculations of the energy band structures of double stranded DNA in the presence of water and Na+ ions. Solid State Communications, 2011, 151, 301-305. | 1.9 | 10 |
| 24 | Modeling laser induced molecule excitation using real-time time-dependent density functional theory: application to 5- and 6-benzyluracil. Physical Chemistry Chemical Physics, 2015, 17, 5861-5871. | 2.8 | 10 |
| 25 | Exploring the Polymorphism of Drostanolone Propionate. Molecules, 2020, 25, 1436. | 3.8 | 10 |
| 26 | Ab initio study of the ammonia-ammonia dimer: BSSE-free structures and intermolecular harmonic vibrational frequencies. International Journal of Quantum Chemistry, 2004, 99, 585-593. | 2.0 | 9 |
| 27 | Dressed Adiabatic and Diabatic Potentials for the Rennerâ€“Teller/Jahnâ€“Teller F + H<sub>2</sub> System. Journal of Physical Chemistry A, 2013, 117, 8497-8505. | 2.5 | 9 |
| 28 | Influence of the sequence on the ab initio band structures of single and double stranded DNA models. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 2157-2162. | 2.1 | 9 |
| 29 | Supramolecular anion recognition by Î²-HCH. Chemical Communications, 2016, 52, 12322-12325. | 4.1 | 9 |
| 30 | Glassy carbon electrode modified with hemin and new melamine compounds for H2O2 amperometric detection. Journal of Solid State Electrochemistry, 2016, 20, 3071-3081. | 2.5 | 9 |
| 31 | The nature of intermolecular interactions in pyridiniumâ€“anionâ€“Î²-hexachlorocyclohexane molecular crystals. Physical Chemistry Chemical Physics, 2017, 19, 20691-20698. | 2.8 | 9 |
| 32 | Circulene covered fullerenes. Computational and Theoretical Chemistry, 2009, 904, 28-34. | 1.5 | 8 |
| 33 | Omega Polynomial in Diamond-like Networks. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 236-243. | 2.1 | 8 |
| 34 | Carbon multi-shell cages. Physical Chemistry Chemical Physics, 2014, 16, 5260. | 2.8 | 8 |
| 35 | Light-induced spin transitions in Ni(II)-based macrocyclic-ligand complexes: A DFT study. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 376, 316-323. | 3.9 | 8 |
| 36 | The role of water and K+ ion in the charge transfer between <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>PO</mml:mtext></mml:mrow><mml:mrow><mml:mn>4</m groups of DNA and the lysine+ and arginine+ side chains of histone proteins. Chemical Physics Letters, 2008, 463, 211-213. | 2.0 | 8 |

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|---|---|---|---|
| 37 | Localization and anharmonicity of the vibrational modes for GC Watsonâ€“Crick and Hoogsteen base pairs. Journal of Molecular Modeling, 2011, 17, 3265-3274. | 1.8 | 7 |
| 38 | Tautomerism and proton transfer in photoionized acetaldehyde and acetaldehydeâ€“water clusters. Journal of Mass Spectrometry, 2014, 49, 700-708. | 1.6 | 7 |
| 39 | Inception of Acetic Acid/Water Cluster Growth in Molecular Beams. ChemPhysChem, 2015, 16, 3021-3029. | 2.1 | 7 |
| 40 | Poly[3,4â€dihydroxybenzhydrazide]: A Polydopamine Analogue?. Macromolecular Chemistry and Physics, 2018, 219, 1700564. | 2.2 | 7 |
| 41 | Dopamine Photochemical Behaviour under UV Irradiation. International Journal of Molecular Sciences, 2022, 23, 5483. | 4.1 | 7 |
| 42 | Hole mobilities of periodic models of DNA double helices in the nucleosomes at different temperatures. Chemical Physics Letters, 2013, 565, 128-131. | 2.6 | 6 |
| 43 | The influence of anharmonic and solvent effects on the theoretical vibrational spectra of the guanineâ€“cytosine base pairs in Watsonâ€“Crick and Hoogsteen configurations. Journal of Molecular Modeling, 2014, 20, 2113. | 1.8 | 6 |
| 44 | Intermolecular Interaction in Methylene Halide (CH2F2, CH2Cl2, CH2Br2 and CH2I2) Dimers. Molecules, 2019, 24, 1810. | 3.8 | 6 |
| 45 | Succinic, fumaric, adipic and oxalic acid cocrystals of promethazine hydrochloride. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 107-119. | 0.5 | 6 |
| 46 | Nitrogen Substituted Phenothiazine Derivatives: Modelling of Molecular Self-Assembling. International Journal of Molecular Sciences, 2011, 12, 3102-3116. | 4.1 | 5 |
| 47 | Study of binary systems of Î²-cyclodextrin with a highly potential anti-mycobacterial drug. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2012, 74, 129-135. | 1.6 | 5 |
| 48 | Improving the Light-Induced Spin Transition Efficiency in Ni(II)-Based Macrocyclic-Ligand Complexes. Molecules, 2019, 24, 4249. | 3.8 | 5 |
| 49 | The Influence of UV Femtosecond Laser Pulses on Bacterial DNA Structure, as Proved by Fourier Transform Infrared (FTâ€IR) Spectroscopy. ChemistrySelect, 2021, 6, 6957-6972. | 1.5 | 5 |
| 50 | Calculation of the hole mobilities of the three homopolynucleotides, poly(guanilic acid), poly(adenilic acid), and polythymidine in the presence of water andNa+ions. Physical Review E, 2008, 78, 061923. | 2.1 | 4 |
| 51 | Charge transfer between DNA and proteins in the nucleosomes. Theoretical Chemistry Accounts, 2010, 125, 185-191. | 1.4 | 4 |
| 52 | Vacuum ultraviolet photoionization and ab initio Investigations of methyl tert-butyl ether (MTBE) clusters and MTBEâ€“water clusters. Chemical Physics Letters, 2013, 561-562, 18-23. | 2.6 | 4 |
| 53 | Theoretical investigation of polymer chain stability in the metal coordinated azorubine and cyclam complex. Chemical Physics, 2015, 457, 152-159. | 1.9 | 4 |
| 54 | UV Photoionization of Sodiumâ€Doped Formic Acid Clusters. ChemPhysChem, 2018, 19, 2724-2734. | 2.1 | 4 |

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|---|---|---|---|
| 55 | Theoretical study of hydrogen bonds between acetylene and selected proton donor systems. International Journal of Quantum Chemistry, 2005, 101, 186-200. | 2.0 | 3 |
| 56 | Ab initio structures of interacting methylene chloride molecules with comparison to the liquid phase. Journal of Molecular Liquids, 2011, 158, 205-207. | 4.9 | 3 |
| 57 | Possible role of ions in DNAâ€“protein interactions in the nucleosomes. Chemical Physics Letters, 2012, 525-526, 115-119. | 2.6 | 3 |
| 58 | Quantum molecular biological investigation of the onset of cancer. International Journal of Quantum Chemistry, 2014, 114, 1229-1235. | 2.0 | 3 |
| 59 | Encasing of Na<sup>+</sup> ion in dimerâ€formed acetic acid clusters. Journal of Mass Spectrometry, 2015, 50, 1136-1143. | 1.6 | 3 |
| 60 | Synthesis, structure, electrochemical behaviour and electrochemical investigations on the assembling with pyrene of a novel C3 cryptand. Supramolecular Chemistry, 2015, 27, 52-58. | 1.2 | 3 |
| 61 | 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, 2018, 14, 1704-1722. | 2.2 | 3 |
| 62 | ITIM distributed grid system applied in high energy, biomolecular and nanotehnology physics. , 2008, , . | | 2 |
| 63 | A simple model for the band structure and D.C. conductivity of an infinite Cï£¾OÂ·Â·Â·Hï£¿N chain perpendicular to the protein backbone. International Journal of Quantum Chemistry, 2009, 109, 612-617. | 2.0 | 2 |
| 64 | Weakly bonded cluster structures of N,Nâ€²-dimethylethyleneurea and water. Journal of Molecular Liquids, 2011, 162, 45-49. | 4.9 | 2 |
| 65 | New p-aminophenol-based dendritic melamines. Iterative synthesis, structure, and electrochemical characterisation. Comptes Rendus Chimie, 2017, 20, 402-414. | 0.5 | 2 |
| 66 | A three-armed cryptand with triazine and pyridine units: synthesis, structure and complexation with polycyclic aromatic compounds. Beilstein Journal of Organic Chemistry, 2018, 14, 1370-1377. | 2.2 | 2 |
| 67 | Synthesis, Structure and Supramolecular Properties of a Novel C3 Cryptand with Pyridine Units in the Bridges. Molecules, 2020, 25, 3789. | 3.8 | 2 |
| 68 | Clusters tagged by alkali metals. AIP Conference Proceedings, 2020, , . | 0.4 | 2 |
| 69 | DFT study of adiabatic singlet-triplet energy gaps in Ni(II)-based macrocyclic-ligand supramolecular complexes. AIP Conference Proceedings, 2020, , . | 0.4 | 2 |
| 70 | Exotic Allotropes of Carbon. Carbon Materials, 2015, , 185-201. | 1.2 | 2 |
| 71 | Theoretical Study of Light-Induced Crosslinking Reaction Between Pyrimidine DNA Bases and Aromatic Amino Acids. Frontiers in Bioengineering and Biotechnology, 2021, 9, 806415. | 4.1 | 2 |
| 72 | Photoionization, Structures, and Energetics of Naâ€Doped Formic Acidâ€“Water Clusters. ChemPhysChem, 2022, 23, . | 2.1 | 2 |

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|---|---|---|---|
| 73 | Complexation of Amlodipine Besylate with Î²-Cyclodextrin. Acta Chimica Slovenica, 2012, 59, 18-23. | 0.6 | 2 |
| 74 | Solvent effect on the anharmonic vibrational frequencies in guanine-cytosine base pair. , 2012, , . | | 1 |
| 75 | Chitosan-based nanocarriers for antimalarials. , 2012, , . | | 1 |
| 76 | Modeling Laser-Induced Molecule Excitations Using Real-Time, Time-Dependent Density Functional Theory. Annual Reports in Computational Chemistry, 2015, 11, 103-146. | 1.7 | 1 |
| 77 | Calculations of electron transfer in the tris[4-(2-thienyl)phenyl]amineâ€“C70 donor-acceptor system. Chemical Physics Letters, 2020, 754, 137654. | 2.6 | 1 |
| 78 | The influence of monovalent and divalent metal cations on the stability of the DNA-protein interaction in the nucleosome core particle. Advances in Quantum Chemistry, 2020, , 269-290. | 0.8 | 1 |
| 79 | Theoretical modeling of the singletâ€“triplet spin transition in different Ni(<scp>ii</scp>)-diketo-pyrphyrin-based metalâ€“ligand octahedral complexes. Physical Chemistry Chemical Physics, 2021, 23, 4784-4795. | 2.8 | 1 |
| 80 | An attempt to synthesize a terthienyl-based analog of indacenedithiophene (IDT): unexpected synthesis of a naphtho[2,3-b]thiophene derivative. RSC Advances, 2021, 11, 9894-9900. | 3.6 | 1 |
| 81 | Energetics of Multi-shell Cages. Carbon Materials, 2013, , 107-119. | 1.2 | 1 |
| 82 | Study of Mixed Clusters of Water and N,N'-dimethylethyleneurea. Ukrainian Journal of Physics, 2022, 56, 796. | 0.2 | 1 |
| 83 | Molecular modeling of the weakly bounded dimers of some phenothiazine derivatives. Journal of Physics: Conference Series, 2009, 182, 012001. | 0.4 | 0 |
| 84 | Model calculation of the specific hole conductivities of three homopolynucleotides, poly(guanilic) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Communications, 2010, 150, 446-449. | 1.9 | 0 |
| 85 | Low-lying excited-states and relaxation pathways of acetophenone. , 2013, , . | | 0 |
| 86 | Low-lying excited states and their relaxation pathways of phenothiazine. AIP Conference Proceedings, 2017, , . | 0.4 | 0 |
| 87 | 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, 2019, 75, 130468. | 1.9 | 0 |
| 88 | "The full mapping of low-lying excited state relaxation dynamic pathways for acetophenone ". Studia Universitatis Babes-Bolyai Chemia, 2021, 66, 239-253. | 0.2 | 0 |