Ioan Baldea

List of Publications by Year in descending order

80 papers	1,748 citations	257357 24 h-index	315616 38 g-index
88 all docs	88 docs citations	88 times ranked	1028 citing authors

#	Article	IF	Citations
1	Are Asymmetric SAMâ€Induced Work Function Modifications Relevant for Real Molecular Rectifiers?. Advanced Theory and Simulations, 2022, 5, .	1.3	4
2	HCnHâ¯ Anion Chains with n â‰¥ 8 Are Nonlinear and Their Permanent Dipole Makes Them Potential Candidates for Astronomical Observation. Molecules, 2022, 27, 3100.	1.7	7
3	Comprehensive Quantum Chemical Characterization of the Astrochemically Relevant HC_nH Chain Family: An Attempt to Aid Astronomical Observations. Advanced Theory and Simulations, 2022, 5, .	1.3	8
4	Quantitative analysis of weak current rectification in molecular tunnel junctions subject to mechanical deformation reveals two different rectification mechanisms for oligophenylene thiolsversusalkane thiols. Nanoscale, 2021, 13, 16755-16768.	2.8	9
5	Why asymmetric molecular coupling to electrodes cannot be at work in real molecular rectifiers. Physical Review B, 2021, 103, .	1.1	12
6	What Can We Learn from the Time Evolution of COVIDâ€19 Epidemic in Slovenia?. Advanced Theory and Simulations, 2021, 4, 2000225.	1.3	1
7	Self-assembled monolayers of oligophenylenes stiffer than steel and silicon, possibly even stiffer than Si3N4. Applied Surface Science Advances, 2021, 5, 100094.	2.9	1
8	Profiling astrophysically relevant MgC4H chains. An attempt to aid astronomical observations. Monthly Notices of the Royal Astronomical Society, 2020, 498, 4316-4326.	1.6	7
9	Suppression of Groups Intermingling as an Appealing Option for Flattening and Delaying the Epidemiological Curve While Allowing Economic and Social Life at a Bearable Level during the COVIDâ€19 Pandemic. Advanced Theory and Simulations, 2020, 3, 2000132.	1.3	7
10	Profiling C4N radicals of astrophysical interest. Monthly Notices of the Royal Astronomical Society, 2020, 493, 2506-2510.	1.6	8
11	Extensive Quantum Chemistry Study of Neutral and Charged C₄N Chains: An Attempt To Aid Astronomical Observations. ACS Earth and Space Chemistry, 2020, 4, 434-448.	1.2	8
12	Evidence That Molecules in Molecular Junctions May Not Be Subject to the Entire External Perturbation Applied to Electrodes. Langmuir, 2020, 36, 1329-1337.	1.6	5
13	A novel route to get functionality in nanoelectronics: Controlling the charge transport by the subtle impact of the coverage of self-assembled monolayers on the conformation of floppy molecules adsorbed on metallic electrodes. Applied Surface Science, 2019, 472, 16-21.	3.1	7
14	Specific issues related to the law of corresponding states for the charge transport in molecular junctions based on graphene electrodes. Applied Surface Science, 2019, 474, 256-261.	3.1	3
15	Alternation of Singlet and Triplet States in Carbonâ€Based Chain Molecules and Its Astrochemical Implications: Results of an Extensive Theoretical Study. Advanced Theory and Simulations, 2019, 2, 1900084.	1.3	19
16	Energy Level Alignment in Molecular Tunnel Junctions by Transport and Spectroscopy: Self-Consistency for the Case of Alkyl Thiols and Dithiols on Ag, Au, and Pt Electrodes. Journal of the American Chemical Society, 2019, 141, 18182-18192.	6.6	68
17	Determination of Energy-Level Alignment in Molecular Tunnel Junctions by Transport and Spectroscopy: Self-Consistency for the Case of Oligophenylene Thiols and Dithiols on Ag, Au, and Pt Electrodes. Journal of the American Chemical Society, 2019, 141, 3670-3681.	6.6	90
18	Impact of molecular conformation on transport and transport-related properties at the nanoscale. Applied Surface Science, 2019, 487, 593-600.	3.1	6

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19	Long Carbon-Based Chains of Interstellar Medium Can Have a Triplet Ground State. Why Is This Important for Astrochemistry?. ACS Earth and Space Chemistry, 2019, 3, 863-872.	1.2	18
20	Mechanical Deformation Distinguishes Tunneling Pathways in Molecular Junctions. Journal of the American Chemical Society, 2019, 141, 497-504.	6.6	21
21	Why one can expect large rectification in molecular junctions based on alkane monothiols and why rectification is so modest. Chemical Science, 2018, 9, 4456-4467.	3.7	49
22	Work function and temperature dependence of electron tunneling through an N-type perylene diimide molecular junction with isocyanide surface linkers. Nanoscale, 2018, 10, 964-975.	2.8	49
23	A sui generis electrode-driven spatial confinement effect responsible for strong twisting enhancement of floppy molecules in closely packed self-assembled monolayers. Physical Chemistry Chemical Physics, 2018, 20, 23492-23499.	1.3	11
24	Vibrational Frequencies of Fractionally Charged Molecular Species: Benchmarking DFT Results against ab Initio Calculations. Journal of Physical Chemistry A, 2017, 121, 2282-2287.	1.1	4
25	Exceptionally Small Statistical Variations in the Transport Properties of Metalâ€“Moleculeâ€“Metal Junctions Composed of 80 Oligophenylene Dithiol Molecules. Journal of the American Chemical Society, 2017, 139, 5696-5699.	6.6	45
26	Protocol for disentangling the thermally activated contribution to the tunneling-assisted charge transport. Analytical results and experimental relevance. Physical Chemistry Chemical Physics, 2017, 19, 11759-11770.	1.3	22
27	Important issues related to the law of corresponding states for the charge transport in molecular junctions with graphene electrodes. Organic Electronics, 2017, 49, 19-23.	1.4	6
28	A surprising way to control the charge transport in molecular electronics: the subtle impact of the coverage of self-assembled monolayers of floppy molecules adsorbed on metallic electrodes. Faraday Discussions, 2017, 204, 35-52.	1.6	12
29	Effect of Heteroatom Substitution on Transport in Alkanedithiol-Based Molecular Tunnel Junctions: Evidence for Universal Behavior. ACS Nano, 2017, 11, 569-578.	7.3	54
30	Probing properties of molecule-based interface systems: general discussion and Discussion of the Concluding Remarks. Faraday Discussions, 2017, 204, 503-530.	1.6	0
31	Supramolecular effects in self-assembled monolayers: general discussion. Faraday Discussions, 2017, 204, 123-158.	1.6	2
32	Preparing macromolecular systems on surfaces: general discussion. Faraday Discussions, 2017, 204, 395-418.	1.6	0
33	Supramolecular systems at liquidâ€“solid interfaces: general discussion. Faraday Discussions, 2017, 204, 271-295.	1.6	2
34	Floppy molecules as candidates for achieving optoelectronic molecular devices without skeletal rearrangement or bond breaking. Physical Chemistry Chemical Physics, 2017, 19, 30842-30851.	1.3	13
35	Vibrational properties of fractionally charged molecules and their relevance for molecular electronics and electrochemistry. Chemical Physics, 2017, 482, 311-318.	0.9	6
36	Invariance of molecular charge transport upon changes of extended molecule size and several related issues. Beilstein Journal of Nanotechnology, 2016, 7, 418-431.	1.5	8

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37	Tuning the conformation of floppy molecules by charge transfer. RSC Advances, 2016, 6, 111903-111907.	1.7	7
38	Fractional molecular charge studied via molecular vibrational properties. Specific aspects in Jahnâ€“Teller active molecular species. RSC Advances, 2016, 6, 93715-93721.	1.7	8
39	Important impact of the experimental platform on the efficient control of electronic and vibrational properties of molecular junctions. International Journal of Nanotechnology, 2016, 13, 685.	0.1	2
40	Uncovering a law of corresponding states for electron tunneling in molecular junctions. Nanoscale, 2015, 7, 10465-10471.	2.8	60
41	Important issues facing model-based approaches to tunneling transport in molecular junctions. Physical Chemistry Chemical Physics, 2015, 17, 20217-20230.	1.3	37
42	An important impact of the moleculeâ€“electrode coupling asymmetry on the efficiency of bias-driven redox processes in molecular junctions. Physical Chemistry Chemical Physics, 2015, 17, 15756-15763.	1.3	13
43	Experimental and Theoretical Analysis of Nanotransport in Oligophenylene Dithiol Junctions as a Function of Molecular Length and Contact Work Function. ACS Nano, 2015, 9, 8022-8036.	7.3	152
44	Counterintuitive issues in the charge transport through molecular junctions. Physical Chemistry Chemical Physics, 2015, 17, 31260-31269.	1.3	18
45	Molecular electronics: general discussion. Faraday Discussions, 2014, 174, 125-151.	1.6	4
46	Organic photovoltaics and energy: general discussion. Faraday Discussions, 2014, 174, 341-355.	1.6	2
47	Quantifying the relative molecular orbital alignment for molecular junctions with similar chemical linkage to electrodes. Nanotechnology, 2014, 25, 455202.	1.3	14
48	Electrochemical setup â€“ a unique chance to simultaneously control orbital energies and vibrational properties of single-molecule junctions with unprecedented efficiency. Physical Chemistry Chemical Physics, 2014, 16, 25942-25949.	1.3	13
49	Concurrent conductance and transition voltage spectroscopy study of scanning tunneling microscopy vacuum junctions. Does it unravel new physics?. RSC Advances, 2014, 4, 33257.	1.7	6
50	Single-Molecule Junctions Based on Bipyridine: Impact of an Unusual Reorganization on Charge Transport. Journal of Physical Chemistry C, 2014, 118, 8676-8684.	1.5	29
51	A quantum chemical study from a molecular transport perspective: ionization and electron attachment energies for species often used to fabricate single-molecule junctions. Faraday Discussions, 2014, 174, 37-56.	1.6	46
52	Transition voltage spectroscopy reveals significant solvent effects on molecular transport and settles an important issue in bipyridine-based junctions. Nanoscale, 2013, 5, 9222.	2.8	47
53	(4,4â€²)-Bipyridinein vacuo and in solvents: a quantum chemical study of a prototypical floppy molecule from a molecular transport perspective. Physical Chemistry Chemical Physics, 2013, 15, 1918-1928.	1.3	35
54	Demonstrating why DFT-calculations for molecular transport in solvents need scissor corrections. Electrochemistry Communications, 2013, 36, 19-21.	2.3	23

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55	Important Insight into Electron Transfer in Single-Molecule Junctions Based on Redox Metalloproteins from Transition Voltage Spectroscopy. Journal of Physical Chemistry C, 2013, 117, 25798-25804.	1.5	37
56	Ambipolar transition voltage spectroscopy: Analytical results and experimental agreement. Physical Review B, 2012, 85, .	1.1	132
57	Transition voltage spectroscopy in vacuum break junction: Possible role of surface states. Europhysics Letters, 2012, 98, 17010.	0.7	24
58	Extending the Newns-Anderson model to allow nanotransport studies through molecules with floppy degrees of freedom. Europhysics Letters, 2012, 99, 47002.	0.7	35
59	Evidence on single-molecule transport in electrostatically-gated molecular transistors. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 1472-1476.	0.9	11
60	Interpretation of Stochastic Events in Single-Molecule Measurements of Conductance and Transition Voltage Spectroscopy. Journal of the American Chemical Society, 2012, 134, 7958-7962.	6.6	52
61	Transition voltage spectroscopy in vacuum break junction: The standard tunneling barrier model and beyond. Physica Status Solidi (B): Basic Research, 2012, 249, 1791-1804.	0.7	17
62	Effects of stochastic fluctuations at moleculeâ€“electrode contacts in transition voltage spectroscopy. Chemical Physics, 2012, 400, 65-71.	0.9	41
63	Transition voltage spectroscopy: Artefacts of the Simmons approach. Journal of Physics and Chemistry of Solids, 2012, 73, 1151-1153.	1.9	8
64	Revealing molecular orbital gating by transition voltage spectroscopy. Chemical Physics, 2010, 377, 15-20.	0.9	39
65	Characterization of assembled quantum dots and singleâ€electron transistors by photoemission and photoabsorption. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, 2671-2674.	0.8	1
66	Sources of negative differential resistance in electric nanotransport. Physical Review B, 2010, 81, .	1.1	25
67	Multi-state vibronic interactions in the fluorobenzene radical cation: The importance of quadratic coupling terms. Chemical Physics, 2007, 338, 207-219.	0.9	43
68	Jahn-Teller and related conical intersections in the benzene radical cation and the monofluoro derivate. Journal of Molecular Structure, 2007, 838, 94-99.	1.8	14
69	Multi-mode vibronic interactions in the five lowest electronic states of the fluorobenzene radical cation. Chemical Physics, 2006, 329, 65-75.	0.9	31
70	Multistate multimode vibronic dynamics: Entanglement of electronic and vibrational degrees of freedom in the benzene radical cation. Journal of Chemical Physics, 2006, 124, 064101.	1.2	32
71	Orbital Picture of Ionization and Its Breakdown in Nanoarrays of Quantum Dots. Physical Review Letters, 2002, 89, 133003.	2.9	13
72	Quantum Phonon Fluctuations in Mesoscopic Dimerized Systems. Journal of the Physical Society of Japan, 1999, 68, 1954-1962.	0.7	8

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73	Structural and magnetic transitions in ensembles of mesoscopic Peierls rings in a magnetic flux. Physical Review B, 1999, 60, 6646-6654.	1.1	7
74	How small can a Peierls dimerized chain be?. Solid State Communications, 1998, 106, 733-737.	0.9	9
75	Finite-size effects and quantum phonon fluctuations in the optical absorption edgeof dimerized chains. Physical Review B, 1997, 55, 1481-1485.	1.1	16
76	Coexistence of short- and large-scale phase variations in a charge-density wave weakly coupled to impurities. Physical Review B, 1995, 52, 11845-11852.	1.1	7
77	Individual versus collective pinning in charge-density-wave systems with impurties. Physical Review B, 1995, 51, 1495-1506.	1.1	9
78	Quasiregular impurity distribution driven by a charge-density wave. Physical Review B, 1993, 48, 8619-8628.	1.1	12
79	On the effect of impurities in the one-dimensional electron-phonon system. Physica Scripta, 1989, 40, 311-314.	1.2	3
80	Exact Analytic Formula for Conductance Predicting a Tunable Sommerfeldâ€“Arrhenius Thermal Transition within a Singleâ€Step Tunneling Mechanism in Molecular Junctions Subject to Mechanical Stretching. Advanced Theory and Simulations, 0, , 2200158.	1.3	3