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List of Publications by Year
in descending order

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52	753	516561	610775
papers	citations	16 h-index	24 g-index

54	54	54	1001
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Shedding light on the binding mechanism of kinase inhibitors BI-2536, Volasetib and Ro-3280 with their pharmacological target PLK1. Journal of Photochemistry and Photobiology B: Biology, 2022, 232, 112477.	1.7	5
2	Fragment dissolved molecular dynamics: a systematic and efficient method to locate binding sites. Physical Chemistry Chemical Physics, 2021, 23, 3123-3134.	1.3	3
3	Triphenylamine- and triazine-containing hydrogen bonded complexes: liquid crystalline supramolecular semiconductors. Journal of Materials Chemistry C, 2021, 9, 1972-1982.	2.7	7
4	Discovery of Diverse Natural Products as Inhibitors of SARS-CoV-2 M^{pro} Protease through Virtual Screening. Journal of Chemical Information and Modeling, 2021, 61, 6094-6106.	2.5	14
5	Molecular Determinants for the Activation/Inhibition of Bak Protein by BH3 Peptides. Journal of Chemical Information and Modeling, 2020, 60, 1632-1643.	2.5	12
6	Crosstalk between hydroxytyrosol, a major olive oil phenol, and HIF-1 in MCF-7 breast cancer cells. Scientific Reports, 2020, 10, 6361.	1.6	26
7	Toward understanding calmodulin plasticity by molecular dynamics. Future Medicinal Chemistry, 2019, 11, 975-991.	1.1	1
8	Effect of set up protocols on the accuracy of alchemical free energy calculation over a set of ACK1 inhibitors. PLoS ONE, 2019, 14, e0213217.	1.1	11
9	A multistep docking and scoring protocol for congeneric series: Implementation on kinase DFG-out type II inhibitors. Future Medicinal Chemistry, 2018, 10, 297-318.	1.1	2
10	Inspecting the Electronic Architecture and Semiconducting Properties of a Rosetteâ€Like Supramolecular Columnar Liquid Crystal. Chemistry - A European Journal, 2018, 24, 17459-17463.	1.7	8
11	Butterfly Molecules: How Cross-Stacking Determines Bulk Physical Properties. Journal of Physical Chemistry C, 2018, 122, 12002-12014.	1.5	12
12	Binding of the anticancer drug BI-2536 to human serum albumin. A spectroscopic and theoretical study. Journal of Photochemistry and Photobiology B: Biology, 2017, 172, 77-87.	1.7	8
13	Effect of five-membered ring and heteroatom substitution on charge transport properties of perylene discotic derivatives: A theoretical approach. Journal of Chemical Physics, 2016, 145, 054903.	1.2	6
14	DFT study of the effect of fluorine atoms on the crystal structure and semiconducting properties of poly(arylene-ethynylene) derivatives. Journal of Chemical Physics, 2016, 144, 154902.	1.2	19
15	A DFT study on the mechanism and kinetics of reactions of pterostilbene with hydroxyl and hydroperoxyl radicals. Computational and Theoretical Chemistry, 2016, 1077, 113-118.	1.1	7
16	DFT Study of the Ambipolar Character of Polymers on the Basis of s-Tetrazine and Aryl Rings. Journal of Physical Chemistry C, 2015, 119, 4588-4599.	1.5	24
17	Bis(arylene-ethynylene)-s-tetrazines: A Promising Family of n-Type Organic Semiconductors?. Journal of Physical Chemistry C, 2015, 119, 18945-18955.	1.5	18
18	A DFT approach to the charge transport related properties in columnar stacked Ï€-conjugated N-heterocycle cores including electron donor and acceptor units. Physical Chemistry Chemical Physics, 2015, 17, 605-618.	1.3	12

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19	Insight into the Binding of DFG-out Allosteric Inhibitors to B-Raf Kinase Using Molecular Dynamics and Free Energy Calculations. Current Computer-Aided Drug Design, 2015, 11, 124-136.	0.8	2
20	Molecular dynamics analysis of the interaction between the human BCL6 BTB domain and its SMRT, NcoR and BCOR corepressors: The quest for a consensus dynamic pharmacophore. Journal of Molecular Graphics and Modelling, 2014, 50, 142-151.	1.3	9
21	Electronic Structure and Charge Transport Properties of a Series of 3,6-(Diphenyl)-s-tetrazine Derivatives: Are They Suitable Candidates for Molecular Electronics?. Journal of Physical Chemistry C, 2014, 118, 26427-26439.	1.5	13
22	Theoretical estimation of the optical bandgap in a series of poly(aryl-ethynylene)s: A DFT study. Journal of Chemical Physics, 2014, 140, 044908.	1.2	16
23	Crystal structure and charge transport properties of poly(arylene-ethynylene) derivatives: A DFT approach. Journal of Chemical Physics, 2013, 138, 154902.	1.2	15
24	Theoretical Approach to the Study of Thiophene-Based Discotic Systems As Organic Semiconductors. Journal of Physical Chemistry C, 2013, 117, 15-22.	1.5	10
25	A Tuned LRC-DFT Design of Ambipolar Diketopyrrolopyrrole-Containing Quinoidal Molecules Interesting for Molecular Electronics. Journal of Chemical Theory and Computation, 2013, 9, 2591-2601.	2.3	10
26	Kinetic and mechanistic study of the atmospheric reaction of MBO331 with Cl atoms. Molecular Physics, 2012, 110, 2941-2950.	0.8	4
27	Electronic properties of diphenyl-s-tetrazine and some related oligomers. An spectroscopic and theoretical study. Chemical Physics, 2012, 408, 17-27.	0.9	16
28	Poly(arylenethynyl-thienoacenes) as candidates for organic semiconducting materials. A DFT insight. Organic Electronics, 2012, 13, 3244-3253.	1.4	24
29	The role of disorder on the electronic structure of conjugated polymers. The case of poly-2,5-bis(phenylethynyl)-1,3,4-thiadiazole. Physical Chemistry Chemical Physics, 2011, 13, 14500.	1.3	14
30	Optoelectronic and Charge Transport Properties of Oligomers Based on Phenylethynylene Units Linked to Thieno-acenes: A DFT Study. Journal of Physical Chemistry C, 2011, 115, 6922-6932.	1.5	31
31	Theoretical Study of the Effect of Alkyl and Alkoxy Lateral Chains on the Structural and Electronic Properties of Ï€-Conjugated Polymers Consisting of Phenylethynyl-1,3,4-thiadiazole. Journal of Physical Chemistry C, 2011, 115, 2865-2873.	1.5	43
32	Predicting binding energies of CDK6 inhibitors in the hit-to-lead process. Theoretical Chemistry Accounts, 2011, 128, 807-823.	0.5	6
33	Does the number of nitrogen atoms have an influence on the conducting properties of diphenylazines? A DFT insight. Chemical Physics, 2011, 379, 51-56.	0.9	7
34	Molecular structure, conformational preferences and vibrational analysis of 2-hydroxystyrene: A computational and spectroscopic research. Chemical Physics, 2010, 374, 62-76.	0.9	3
35	The Role of Linear Alkyl and Alkoxy Side Chains in the Modulation of the Structure and Electrical Properties of Bithiophene:a Theoretical Study. Australian Journal of Chemistry, 2010, 63, 1297.	0.5	6
36	Density functional theory study of the optical and electronic properties of oligomers based on phenyl-ethynyl units linked to triazole, thiadiazole, and oxadiazole rings to be used in molecular electronics. Journal of Chemical Physics, 2010, 132, 064901.	1.2	29

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37	Molecular conductivity switching of two benzene rings under electric field. Applied Physics Letters, 2010, 97, 262114.	1.5	22
38	Theoretical Study of Bis(phenylethynyl)thienoacenes as Precursors of Molecular Wires for Molecular Electronics. Journal of Physical Chemistry C, 2010, 114, 12325-12334.	1.5	19
39	Theoretical study of the effect of ethynyl group on the structure and electrical properties of phenyl-thiadiazole systems as precursors of electron-conducting materials. Journal of Chemical Physics, 2009, 130, 234907.	1.2	30
40	A quantum mechanical study on polymer flexibility: Extended model from monomer to tetramer of 2- and 4-bromostyrenes. Polymer, 2009, 50, 317-327.	1.8	9
41	New insight into the structure, internal rotation barrier and vibrational analysis of 2-fluorostyrene. Chemical Physics, 2009, 361, 94-105.	0.9	4
42	Recognition and discrimination of DNA quadruplexes by acridine-peptide conjugates. Organic and Biomolecular Chemistry, 2009, 7, 76-84.	1.5	60
43	Proteinâ€“protein recognition as a first step towards the inhibition of XIAP and Survivin antiâ€apoptotic proteins. Journal of Molecular Recognition, 2008, 21, 190-204.	1.1	20
44	Molecular Structure, Vinyl Rotation Barrier, and Vibrational Dynamics of 2,6-Dichlorostyrene. A Theoretical and Experimental Research. Journal of Physical Chemistry A, 2007, 111, 6406-6419.	1.1	3
45	Exploring the Recognition of Quadruplex DNA by an Engineered Cys2-His2Zinc Finger Proteinâ€. Biochemistry, 2006, 45, 1393-1399.	1.2	37
46	The molecular structure and vibrational spectrum of 4-chlorostyrene. Journal of Molecular Structure, 2006, 789, 118-127.	1.8	4
47	Weak Câ€“Hâ‹¯O and Câ€“Hâ‹¯Ï€ hydrogen bonds in crystal 1-indanone. An structural and spectroscopic analysis. Journal of Molecular Structure, 2004, 707, 33-46.	1.8	11
48	An approach to the structure and vibrational analysis of cis- and trans-3-chlorostyrene through IR/Raman and INS spectroscopies and theoretical ab initio/DFT calculations. Physical Chemistry Chemical Physics, 2004, 6, 1133-1143.	1.3	10
49	Tetrapeptides induce selective recognition for G-quadruplexes when conjugated to a DNA-binding platform. Organic and Biomolecular Chemistry, 2004, 2, 2925.	1.5	36
50	The vibrational analysis of styrene, revisited. Chemical Physics Letters, 2003, 372, 255-262.	1.2	19
51	The molecular force field of 4-fluorostyrene: an insight into its vibrational analysis using inelastic neutron scattering, optical spectroscopies (IR/Raman) and theoretical calculationsElectronic supplementary information (ESI) available: Structural parameters, frequences and force constants of 4-fluorostyrene (4 tables); observed and calculated IR spectra and INS spectra (6 figures). See http://www.rsc.org/suppdata/cp/b2/b212620f/. Physical Chemistry Chemical Physics, 2003, 5, 1760-1768.	1.3	7
52	Refined, scaled and canonical force fields for the cis- and trans-3-fluorostyrene conformers. An interplay between theoretical calculations, IR/Raman and INS data. Physical Chemistry Chemical Physics, 2002, 4, 4890-4901.	1.3	8