Grzegorz Mazur

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1054976/publications.pdf

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20	596	840776 11	794594 19
papers	citations	h-index	g-index

20	20	20	716
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Soft Selection Rules for Femtosecond Pumpâ€“Probe Vibrational Coherence Spectroscopy. Journal of Physical Chemistry C, 2020, 124, 23501-23510.	3.1	2
2	Partial atomic multipoles for internally consistent microelectrostatic calculations. Journal of Computational Chemistry, 2017, 38, 2420-2429.	3.3	0
3	Boys function evaluation on graphical processing units. Journal of Mathematical Chemistry, 2016, 54, 2022-2047.	1.5	4
4	Automatic code generation for quantum chemistry applications. International Journal of Quantum Chemistry, 2016, 116, 1370-1381.	2.0	4
5	Automatized Parameterization of DFTB Using Particle Swarm Optimization. Journal of Chemical Theory and Computation, 2016, 12, 53-64.	5.3	55
6	Automatized Parameterization of the Densityâ€functional Tightâ€binding Method. II. Twoâ€center Integrals. Journal of the Chinese Chemical Society, 2016, 63, 57-68.	1.4	13
7	Charge-Transfer States in Pentacene: Dimer versus Crystal. Journal of Physical Chemistry C, 2015, 119, 14338-14342.	3.1	24
8	A uniform approach to the description of multicenter bonding. Physical Chemistry Chemical Physics, 2014, 16, 20514-20523.	2.8	112
9	Transition dipole moments of charge transfer excitations in one-component molecular crystals. Chemical Physics, 2012, 397, 92-97.	1.9	6
10	A neural-network controlled dynamic evolutionary scheme for global molecular geometry optimization. International Journal of Applied Mathematics and Computer Science, 2011, 21, 559-566.	1.5	9
11	Time-dependent density functional theory gradients in the Amsterdam density functional package: geometry optimizations of spin-flip excitations. Theoretical Chemistry Accounts, 2011, 129, 331-342.	1.4	48
12	Dressed TDDFT study of lowâ€lying electronic excited states in selected linear polyenes and diphenylopolyenes. International Journal of Quantum Chemistry, 2011, 111, 819-825.	2.0	27
13	Application of the dressed timeâ€dependent density functional theory for the excited states of linear polyenes. Journal of Computational Chemistry, 2009, 30, 811-817.	3.3	56
14	An improved SCPF scheme for polarization energy calculations. Journal of Computational Chemistry, 2008, 29, 988-993.	3.3	3
15	Theoretical calculations of the electroabsorption spectra of perylenetetracarboxylic dianhydride. Journal of Chemical Physics, 2003, 118, 1423-1432.	3.0	32
16	Charge transfer excitons in perylenetetracarboxylic dianhydride â€“ microelectrostatic calculations. Chemical Physics Letters, 2000, 324, 161-165.	2.6	21
17	Quantum chemical results as input for solid state calculations: charge transfer states in molecular crystals. Computational and Theoretical Chemistry, 2000, 527, 91-102.	1.5	36
18	Charge-pair states in organic molecular crystals: localized vs. delocalized description. Synthetic Metals, 2000, 109, 73-77.	3.9	3

#	Article	IF	Citations
19	Band gap and binding energies of charge-transfer excitons in organic molecular crystals. Chemical Physics Letters, 1999, 301, 223-227.	2.6	11
20	Quantum chemical valence indices from the one-determinantal difference approach. Canadian Journal of Chemistry, 1996, 74, 1121-1130.	1.1	130