PÃ©ter R Nagy

List of Publications by Year
in descending order

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49 papers	1,534 citations	430874 18 h-index	315739 38 g-index
49 all docs	49 docs citations	49 times ranked	1417 citing authors

#	Article	IF	Citations
1	The MRCC program system: Accurate quantum chemistry from water to proteins. Journal of Chemical Physics, 2020, 152, 074107.	3.0	264
2	Catalytic Hydrogenation with Frustrated Lewis Pairs: Selectivity Achieved by Sizeâ€Exclusion Design of Lewis Acids. Chemistry - A European Journal, 2012, 18, 574-585.	3.3	151
3	Approaching the Basis Set Limit of CCSD(T) Energies for Large Molecules with Local Natural Orbital Coupled-Cluster Methods. Journal of Chemical Theory and Computation, 2019, 15, 5275-5298.	5.3	112
4	Optimization of the Linear-Scaling Local Natural Orbital CCSD(T) Method: Improved Algorithm and Benchmark Applications. Journal of Chemical Theory and Computation, 2018, 14, 4193-4215.	5.3	94
5	Exact density functional and wave function embedding schemes based on orbital localization. Journal of Chemical Physics, 2016, 145, .	3.0	80
6	An Integral-Direct Linear-Scaling Second-Order MÃ¸llerâ€“Plesset Approach. Journal of Chemical Theory and Computation, 2016, 12, 4897-4914.	5.3	72
7	Optimization of the linear-scaling local natural orbital CCSD(T) method: Redundancy-free triples correction using Laplace transform. Journal of Chemical Physics, 2017, 146, 214106.	3.0	70
8	Tree Tensor Network State with Variable Tensor Order: An Efficient Multireference Method for Strongly Correlated Systems. Journal of Chemical Theory and Computation, 2015, 11, 1027-1036.	5.3	62
9	Interactions between large molecules pose a puzzle for reference quantum mechanical methods. Nature Communications, 2021, 12, 3927.	12.8	57
10	Reduced-cost linear-response CC2 method based on natural orbitals and natural auxiliary functions. Journal of Chemical Physics, 2017, 146, 194102.	3.0	47
11	Integral-Direct and Parallel Implementation of the CCSD(T) Method: Algorithmic Developments and Large-Scale Applications. Journal of Chemical Theory and Computation, 2020, 16, 366-384.	5.3	46
12	Effects of disinfection and sterilization on the dimensional changes and mechanical properties of 3D printed surgical guides for implant therapy â€“ pilot study. BMC Oral Health, 2020, 20, 19.	2.3	44
13	Perspectives of APSGâ€based multireference perturbation theories. International Journal of Quantum Chemistry, 2014, 114, 1048-1052.	2.0	39
14	Reduced-cost second-order algebraic-diagrammatic construction method for excitation energies and transition moments. Journal of Chemical Physics, 2018, 148, .	3.0	37
15	Accurate Reduced-Cost CCSD(T) Energies: Parallel Implementation, Benchmarks, and Large-Scale Applications. Journal of Chemical Theory and Computation, 2021, 17, 860-878.	5.3	32
16	Stereocontrol in Diphenylprolinol Silyl Ether Catalyzed Michael Additions: Steric Shielding or Curtinâ€“Hammett Scenario?. Journal of the American Chemical Society, 2017, 139, 17052-17063.	13.7	29
17	Dual Basis Set Approach for Density Functional and Wave Function Embedding Schemes. Journal of Chemical Theory and Computation, 2018, 14, 4600-4615.	5.3	29
18	Investigation of the mechanical and chemical characteristics of nanotubular and nano-pitted anodic films on grade 2 titanium dental implant materials. Materials Science and Engineering C, 2017, 78, 69-78.	7.3	24

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19	Size-consistent explicitly correlated triple excitation correction. Journal of Chemical Physics, 2021, 155, 034107.	3.0	19
20	Reduced-Scaling Correlation Methods for the Excited States of Large Molecules: Implementation and Benchmarks for the Second-Order Algebraic-Diagrammatic Construction Approach. Journal of Chemical Theory and Computation, 2019, 15, 6111-6126.	5.3	18
21	Linear-Scaling Open-Shell MP2 Approach: Algorithm, Benchmarks, and Large-Scale Applications. Journal of Chemical Theory and Computation, 2021, 17, 2886-2905.	5.3	16
22	Chemical etching of nitinol stents. Acta of Bioengineering and Biomechanics, 2013, 15, 3-8.	0.4	16
23	Injection Molding of Degradable Interference Screws into Polymeric Mold. Materials Science Forum, 2010, 659, 73-77.	0.3	15
24	Octylphenol and Nonylphenol in Surface Water of RÃ¡ckevei-SoroksÃ¡ri Danube Branch, Hungary. Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering, 2005, 40, 1679-1688.	1.7	14
25	Spin Component Scaling in Multiconfiguration Perturbation Theory. Journal of Physical Chemistry A, 2011, 115, 523-534.	2.5	13
26	Mayerâ€™s orthogonalization: relation to the Gram-Schmidt and LÃ¶wdinâ€™s symmetrical scheme. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	12
27	The role of ultimate elongation in the determination of valid ligament range of essential work of fracture tests. Journal of Materials Science, 2012, 47, 2228-2233.	3.7	12
28	Polycyclic aromatic hydrocarbons (PAHs) in surface waters of RÃ¡ckevei-SoroksÃ¡ri Danube Branch, Hungary. Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering, 2007, 42, 231-240.	1.7	11
29	Transferable interactions of Li+ and Mg2+ ions in polarizable models. Journal of Chemical Physics, 2020, 153, 104113.	3.0	11
30	Improved description of ligand polarization enhances transferability of ionâ€“ligand interactions. Journal of Chemical Physics, 2020, 153, 094115.	3.0	11
31	Characterization of the fracture properties of aragoniteâ€•and calciteâ€filled poly(Ìµâ€caprolactone) by the essential work of fracture method. Journal of Applied Polymer Science, 2011, 120, 2587-2595.	2.6	9
32	Resonance Raman Optical Activity of Single Walled Chiral Carbon Nanotubes. Journal of Physical Chemistry A, 2016, 120, 5527-5538.	2.5	9
33	Unitary perturbation theory applied to multiconfigurational reference functions. International Journal of Quantum Chemistry, 2013, 113, 230-238.	2.0	8
34	Novel orthogonalization and biorthogonalization algorithms. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	7
35	Basis set truncation corrections for improved frozen natural orbital CCSD(T) energies. Molecular Physics, 2021, 119, .	1.7	7
36	Essential work of fracture study of polymers: a novel criterion for the validation of tested ligament range. Journal of Materials Science, 2011, 46, 7901-7904.	3.7	6

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37	Theoretical vibrational optical activity of chiral carbon nanoparticles: Fullerenes and carbon nanotubes. Physica Status Solidi (B): Basic Research, 2014, 251, 2451-2456.	1.5	6
38	Vibrational optical activity of chiral carbon nanoclusters treated by a generalized Ï€-electron method. Journal of Chemical Physics, 2014, 140, 044112.	3.0	5
39	Methylâ€Induced Polarization Destabilizes the Noncovalent Interactions of Nâ€Methylated Lysines. Chemistry - A European Journal, 2021, 27, 11005-11014.	3.3	5
40	Investigating the Time Dependent Behavior of Thermoplastic Polymers under Tensile Load. Macromolecular Symposia, 2006, 239, 176-181.	0.7	4
41	Development of Nitinol Stents: Electropolishing Experiments. Materials Science Forum, 2012, 729, 436-441.	0.3	3
42	Control of wind power. , 2013, , .		3
43	Monofluorinated Polycyclic Aromatic Hydrocarbons: Surrogate Standards for HPLC Analysis of Surface Water and Sediment Samples. Journal of Liquid Chromatography and Related Technologies, 2007, 31, 240-249.	1.0	2
44	Laser Cutting of Small Diameter Nitinol Tube. Materials Science Forum, 2012, 729, 460-463.	0.3	2
45	Development of Nitinol Stents: Etching Experiments. Materials Science Forum, 2012, 729, 240-245.	0.3	1
46	Stent Retention Measurement. Materials Science Forum, 0, 659, 283-288.	0.3	0
47	Limitations of the rotor voltage of doubly fed induction generator in shaping the slip-torque characteristics. , 2014, , .		0
48	Chemical Etching of Ultrafine Grained Titanium Surfaces to Optimise Cell Attachment. Materials Science Forum, 0, 812, 265-270.	0.3	0
49	Direction-dependent secondary bonds and their stepwise melting in a uracil-based molecular crystal studied by infrared spectroscopy and theoretical modeling. Chemical Physics Letters, 2018, 691, 163-168.	2.6	0