

# PÃ©ter R Nagy

## List of Publications by Year in descending order

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49  
papers

1,534  
citations

489802

18  
h-index

355658

38  
g-index

49  
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49  
docs citations

49  
times ranked

1579  
citing authors

#	ARTICLE	IF	CITATIONS
1	Accurate Reduced-Cost CCSD(T) Energies: Parallel Implementation, Benchmarks, and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 860-878.	2.3	32
2	Linear-Scaling Open-Shell MP2 Approach: Algorithm, Benchmarks, and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2886-2905.	2.3	16
3	Interactions between large molecules pose a puzzle for reference quantum mechanical methods. <i>Nature Communications</i> , 2021, 12, 3927.	5.8	57
4	MethylŃ-induced Polarization Destabilizes the Noncovalent Interactions of NŃ-methylated Lysines. <i>Chemistry - A European Journal</i> , 2021, 27, 11005-11014.	1.7	5
5	Size-consistent explicitly correlated triple excitation correction. <i>Journal of Chemical Physics</i> , 2021, 155, 034107.	1.2	19
6	Basis set truncation corrections for improved frozen natural orbital CCSD(T) energies. <i>Molecular Physics</i> , 2021, 119, .	0.8	7
7	Integral-Direct and Parallel Implementation of the CCSD(T) Method: Algorithmic Developments and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 366-384.	2.3	46
8	Transferable interactions of Li <sup>+</sup> and Mg <sup>2+</sup> ions in polarizable models. <i>Journal of Chemical Physics</i> , 2020, 153, 104113.	1.2	11
9	Improved description of ligand polarization enhances transferability of ionŃligand interactions. <i>Journal of Chemical Physics</i> , 2020, 153, 094115.	1.2	11
10	The MRCC program system: Accurate quantum chemistry from water to proteins. <i>Journal of Chemical Physics</i> , 2020, 152, 074107.	1.2	264
11	Effects of disinfection and sterilization on the dimensional changes and mechanical properties of 3D printed surgical guides for implant therapy Ń pilot study. <i>BMC Oral Health</i> , 2020, 20, 19.	0.8	44
12	Approaching the Basis Set Limit of CCSD(T) Energies for Large Molecules with Local Natural Orbital Coupled-Cluster Methods. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5275-5298.	2.3	112
13	Reduced-Scaling Correlation Methods for the Excited States of Large Molecules: Implementation and Benchmarks for the Second-Order Algebraic-Diagrammatic Construction Approach. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6111-6126.	2.3	18
14	Reduced-cost second-order algebraic-diagrammatic construction method for excitation energies and transition moments. <i>Journal of Chemical Physics</i> , 2018, 148, .	1.2	37
15	Direction-dependent secondary bonds and their stepwise melting in a uracil-based molecular crystal studied by infrared spectroscopy and theoretical modeling. <i>Chemical Physics Letters</i> , 2018, 691, 163-168.	1.2	0
16	Optimization of the Linear-Scaling Local Natural Orbital CCSD(T) Method: Improved Algorithm and Benchmark Applications. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4193-4215.	2.3	94
17	Dual Basis Set Approach for Density Functional and Wave Function Embedding Schemes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4600-4615.	2.3	29
18	Investigation of the mechanical and chemical characteristics of nanotubular and nano-pitted anodic films on grade 2 titanium dental implant materials. <i>Materials Science and Engineering C</i> , 2017, 78, 69-78.	3.8	24

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19	Reduced-cost linear-response CC2 method based on natural orbitals and natural auxiliary functions. <i>Journal of Chemical Physics</i> , 2017, 146, 194102.	1.2	47
20	Stereocontrol in Diphenylprolinol Silyl Ether Catalyzed Michael Additions: Steric Shielding or Curtinâ€“Hammett Scenario?. <i>Journal of the American Chemical Society</i> , 2017, 139, 17052-17063.	6.6	29
21	Optimization of the linear-scaling local natural orbital CCSD(T) method: Redundancy-free triples correction using Laplace transform. <i>Journal of Chemical Physics</i> , 2017, 146, 214106.	1.2	70
22	Exact density functional and wave function embedding schemes based on orbital localization. <i>Journal of Chemical Physics</i> , 2016, 145, .	1.2	80
23	An Integral-Direct Linear-Scaling Second-Order MÅ  lerâ€“Plesset Approach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4897-4914.	2.3	72
24	Resonance Raman Optical Activity of Single Walled Chiral Carbon Nanotubes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5527-5538.	1.1	9
25	Tree Tensor Network State with Variable Tensor Order: An Efficient Multireference Method for Strongly Correlated Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1027-1036.	2.3	62
26	Novel orthogonalization and biorthogonalization algorithms. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	7
27	Vibrational optical activity of chiral carbon nanoclusters treated by a generalized i€-electron method. <i>Journal of Chemical Physics</i> , 2014, 140, 044112.	1.2	5
28	Limitations of the rotor voltage of doubly fed induction generator in shaping the slip-torque characteristics. , 2014, , .		0
29	Theoretical vibrational optical activity of chiral carbon nanoparticles: Fullerenes and carbon nanotubes. <i>Physica Status Solidi (B): Basic Research</i> , 2014, 251, 2451-2456.	0.7	6
30	Perspectives of APSCâ€“based multireference perturbation theories. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1048-1052.	1.0	39
31	Unitary perturbation theory applied to multiconfigurational reference functions. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 230-238.	1.0	8
32	Control of wind power. , 2013, , .		3
33	Chemical etching of nitinol stents. <i>Acta of Bioengineering and Biomechanics</i> , 2013, 15, 3-8.	0.2	16
34	Laser Cutting of Small Diameter Nitinol Tube. <i>Materials Science Forum</i> , 2012, 729, 460-463.	0.3	2
35	Development of Nitinol Stents: Electropolishing Experiments. <i>Materials Science Forum</i> , 2012, 729, 436-441.	0.3	3
36	Development of Nitinol Stents: Etching Experiments. <i>Materials Science Forum</i> , 2012, 729, 240-245.	0.3	1

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37	Catalytic Hydrogenation with Frustrated Lewis Pairs: Selectivity Achieved by Size-Exclusion Design of Lewis Acids. <i>Chemistry - A European Journal</i> , 2012, 18, 574-585.	1.7	151
38	Mayer's orthogonalization: relation to the Gram-Schmidt and Löwdin's symmetrical scheme. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	12
39	The role of ultimate elongation in the determination of valid ligament range of essential work of fracture tests. <i>Journal of Materials Science</i> , 2012, 47, 2228-2233.	1.7	12
40	Spin Component Scaling in Multiconfiguration Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2011, 115, 523-534.	1.1	13
41	Essential work of fracture study of polymers: a novel criterion for the validation of tested ligament range. <i>Journal of Materials Science</i> , 2011, 46, 7901-7904.	1.7	6
42	Characterization of the fracture properties of aragonite- and calcite-filled poly( $\epsilon$ -caprolactone) by the essential work of fracture method. <i>Journal of Applied Polymer Science</i> , 2011, 120, 2587-2595.	1.3	9
43	Injection Molding of Degradable Interference Screws into Polymeric Mold. <i>Materials Science Forum</i> , 2010, 659, 73-77.	0.3	15
44	Polycyclic aromatic hydrocarbons (PAHs) in surface waters of Ráckevei-Soroksári Danube Branch, Hungary. <i>Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering</i> , 2007, 42, 231-240.	0.9	11
45	Monofluorinated Polycyclic Aromatic Hydrocarbons: Surrogate Standards for HPLC Analysis of Surface Water and Sediment Samples. <i>Journal of Liquid Chromatography and Related Technologies</i> , 2007, 31, 240-249.	0.5	2
46	Investigating the Time Dependent Behavior of Thermoplastic Polymers under Tensile Load. <i>Macromolecular Symposia</i> , 2006, 239, 176-181.	0.4	4
47	Octylphenol and Nonylphenol in Surface Water of Ráckevei-Soroksári Danube Branch, Hungary. <i>Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering</i> , 2005, 40, 1679-1688.	0.9	14
48	Stent Retention Measurement. <i>Materials Science Forum</i> , 0, 659, 283-288.	0.3	0
49	Chemical Etching of Ultrafine Grained Titanium Surfaces to Optimise Cell Attachment. <i>Materials Science Forum</i> , 0, 812, 265-270.	0.3	0