# 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 | 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 |
| 2 | 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 |
| 3 | Interactions between large molecules pose a puzzle for reference quantum mechanical methods. Nature Communications, 2021, 12, 3927. | 12.8 | 57 |
| 4 | Methylâ€Induced Polarization Destabilizes the Noncovalent Interactions of Nâ€Methylated Lysines. Chemistry - A European Journal, 2021, 27, 11005-11014. | 3.3 | 5 |
| 5 | Size-consistent explicitly correlated triple excitation correction. Journal of Chemical Physics, 2021, 155, 034107. | 3.0 | 19 |
| 6 | Basis set truncation corrections for improved frozen natural orbital CCSD(T) energies. Molecular Physics, 2021, 119, . | 1.7 | 7 |
| 7 | 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 |
| 8 | Transferable interactions of Li+ and Mg2+ ions in polarizable models. Journal of Chemical Physics, 2020, 153, 104113. | 3.0 | 11 |
| 9 | Improved description of ligand polarization enhances transferability of ionâ€“ligand interactions. Journal of Chemical Physics, 2020, 153, 094115. | 3.0 | 11 |
| 10 | The MRCC program system: Accurate quantum chemistry from water to proteins. Journal of Chemical Physics, 2020, 152, 074107. | 3.0 | 264 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 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 | 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 |
| 16 | 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 |
| 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 | Reduced-cost linear-response CC2 method based on natural orbitals and natural auxiliary functions. Journal of Chemical Physics, 2017, 146, 194102. | 3.0 | 47 |
| 20 | 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 |
| 21 | 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 |
| 22 | Exact density functional and wave function embedding schemes based on orbital localization. Journal of Chemical Physics, 2016, 145, . | 3.0 | 80 |
| 23 | An Integral-Direct Linear-Scaling Second-Order MÃ¸llerâ€“Plesset Approach. Journal of Chemical Theory and Computation, 2016, 12, 4897-4914. | 5.3 | 72 |
| 24 | Resonance Raman Optical Activity of Single Walled Chiral Carbon Nanotubes. Journal of Physical Chemistry A, 2016, 120, 5527-5538. | 2.5 | 9 |
| 25 | 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 |
| 26 | Novel orthogonalization and biorthogonalization algorithms. Theoretical Chemistry Accounts, 2015, 134, 1. | 1.4 | 7 |
| 27 | Vibrational optical activity of chiral carbon nanoclusters treated by a generalized Ï€-electron method. Journal of Chemical Physics, 2014, 140, 044112. | 3.0 | 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. Physica Status Solidi (B): Basic Research, 2014, 251, 2451-2456. | 1.5 | 6 |
| 30 | Perspectives of APSGâ€based multireference perturbation theories. International Journal of Quantum Chemistry, 2014, 114, 1048-1052. | 2.0 | 39 |
| 31 | Unitary perturbation theory applied to multiconfigurational reference functions. International Journal of Quantum Chemistry, 2013, 113, 230-238. | 2.0 | 8 |
| 32 | Control of wind power. , 2013, , . | | 3 |
| 33 | Chemical etching of nitinol stents. Acta of Bioengineering and Biomechanics, 2013, 15, 3-8. | 0.4 | 16 |
| 34 | Laser Cutting of Small Diameter Nitinol Tube. Materials Science Forum, 2012, 729, 460-463. | 0.3 | 2 |
| 35 | Development of Nitinol Stents: Electropolishing Experiments. Materials Science Forum, 2012, 729, 436-441. | 0.3 | 3 |
| 36 | Development of Nitinol Stents: Etching Experiments. Materials Science Forum, 2012, 729, 240-245. | 0.3 | 1 |

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|---|---|---|---|
| 37 | 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 |
| 38 | Mayerâ€™s orthogonalization: relation to the Gram-Schmidt and LÃ¶wdinâ€™s symmetrical scheme. Theoretical Chemistry Accounts, 2012, 131, 1. | 1.4 | 12 |
| 39 | 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 |
| 40 | Spin Component Scaling in Multiconfiguration Perturbation Theory. Journal of Physical Chemistry A, 2011, 115, 523-534. | 2.5 | 13 |
| 41 | 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 |
| 42 | Characterization of the fracture properties of aragoniteâ€•and calciteâ€filled poly(Îµâ€caprolactone) by the essential work of fracture method. Journal of Applied Polymer Science, 2011, 120, 2587-2595. | 2.6 | 9 |
| 43 | Injection Molding of Degradable Interference Screws into Polymeric Mold. Materials Science Forum, 2010, 659, 73-77. | 0.3 | 15 |
| 44 | 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 |
| 45 | 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 |
| 46 | Investigating the Time Dependent Behavior of Thermoplastic Polymers under Tensile Load. Macromolecular Symposia, 2006, 239, 176-181. | 0.7 | 4 |
| 47 | 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 |
| 48 | Stent Retention Measurement. Materials Science Forum, 0, 659, 283-288. | 0.3 | 0 |
| 49 | Chemical Etching of Ultrafine Grained Titanium Surfaces to Optimise Cell Attachment. Materials Science Forum, 0, 812, 265-270. | 0.3 | 0 |