PÉTER NAGY

head of Molecular Quantum Simulation ERC Research Group
webpage: www.fkt.bme.hu/~theoreticalchem
e-mail: nagy.peter@vbk.bme.hu, nagyrpeter@gmail.com
address: Budapest University Of Technology And Economics (BME),
Department of Physical Chemistry and Materials Science
H-1111, Budapest, Műegyetem rkp. 3, Hungary

Education

2015 Ph.D. in Theoretical Chemistry, summa cum laude, Eötvös Loránd University (ELTE)
Dissertation: Theoretical developments and computational studies in chiroptical spectroscopies
2011 Master's Degree in Chemistry with honors, ELTE
Thesis: Novel perturbation and orthogonalization methods applied in quantum chemistry
2009 Bachelor's Degree in Chemistry with honors, ELTE
Thesis: Spin-component scaling in multiconfiguration perturbation theory (in Hungarian)

Current and previous positions

2023- research associate professor, Department of Physical Chemistry and Materials Science, BME
2018-2022 research assistant professor, Department of Physical Chemistry and Materials Science, BME
2015-2017 postdoctoral fellow, Quantum Chemistry Research Group, Hungarian Academy of Sciences (HAS)

Grants and fellowships

2023-2028 European Research Council, **ERC Starting grant** (1.175 M€, 30 European chemist per year)
2023-2026 János Bolyai Fellowship of HAS (repeated award only for 2 chemists per year under age 45)
2022-2026 Hungarian Research Fund (HRF, NRDI) young researcher grant (OTKA FK, 105 k€, 10 chemist/year)
2019, 2021 Partnership for Advanced Computing in Europe grants (PRACE, 7.4 & 10.9 million hours)
2018-2021 János Bolyai Fellowship of HAS (awarded to 12 chemists per year under age 45)
2015-2022 Research Scholarship for Young Talents of the Hungarian Nation (3x 1-year projects)
2017-2023 Fellowship of New National Excellence Program (5x 1-year projects)
2006-2014 Membership of the Bolyai College (excellence college of ELTE, 1-2 chemists per class)
2010 Erasmus mobility scholarship (1 semester), University of Leeds

Awards and prizes

2023 Junior Polányi Prize of HAS (**1 prize in physical-chemistry per year under age 35**)
2023 Youth Academic Award of HAS (**2 in chemistry per year under age 35**)
2022 Bolyai Plaquette for best results among János Bolyai Fellows (**1 chemist per year under age 45**)
2020 Junior Prima Prize (6 k€, awarded to ∼1 chemist per year under age 33 by the HAS)
2011 Pro Scientia Gold Medal (awarded to 1-2 chemistry students per year in Hungary)
2011 Master's Degree Excellence award of the Hungarian Chemical Society (∼10 chemists per year)
2009, 2011 2nd & 1st prize at the National Scientific Student's Association Conference of Hungary (OTDK)
2008-2010 Excellence Scholarship of the Republic of Hungary and the Faculty of Sciences, ELTE
2006 Bronze medal winner, 38th International Chemistry Olympiad (IChO), South Korea
2005 Metropolis award: many top 3 places in high-school national competitions (maths, phys, chem)

Supervision of students and postdoctoral fellows

3 postdoctoral associates, 3 Ph.D. students, 3 Master's and 1 Bachelor's students (2x 1st and 1x 2nd prize in national TDK, 2x 1st and 1x 2nd prize in faculty level TDK, 2 ÚKNP scholarship, 1 PhD student excellence scholarship), co-supervisor/consultant in sub-projects of 4 more Ph.D. students at BME

Teaching experience

2015- Physical Chemistry (reaction kinetics, electrochemistry) BME, 16 semesters

2011-2014 Advanced Mathematics and Quantum Mechanics for Chemists, ELTE, 2x3 semesters

Scientific community service

organizer: CECAM Workshop: Non-Covalent Interactions in Large Molecules and Extended Materials
member: Physical Chemistry Final Exam and Scientific Student's Conference Panels at BME (2018-)
HAS Materials and Molecular Structure Committee (2018-)
lecturer: national training program for International Chemistry Olympiad, IChO (6 years)
reviewer: ➤ J. Phys. Chem. Lett., J. Chem. Theory Comput., J. Chem. Phys., J. Phys. Chem. A, Natl. Sci. Rev., J. Mol. Structure (THEOCHEM), J. Mol. Model., J. Math. Chem., Struct. Chem., Mol. Phys., Chem. Phys. Lett.
➤ grant proposals: National Science Centre (Poland), CELSA, HAS, HRF/NRDI
➤ 3 Bachelor's and 3 Master's theses, and 1 Ph.D. dissertation
committee member: 1 Master's and 4 Ph.D. theses defenses

Selected conference participation

Invited talk: European Seminar on Computational Methods in Quantum Chemistry, Copenhagen, 2024
Invited talk and session chair: Quantum International Frontiers, Lodz, 2023
Invited talk: Quantum Chemistry Methods for Materials Science, CECAM workshop, Lausanne, 2022
Talk and organization: Non-Covalent Interactions in Large Molecules and Extended Materials, CECAM workshop, Lausanne, 2021
Contributed talks: Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Vancouver 2022 and Munich 2017 (cca. 25% of the applications were selected)
Invited talk: Central European Symposium on Theoretical Chemistry, Wisla, Poland, 2017
Invited talk: Seminar of Institut für Theoretische Chemie, Stuttgart, 2017

Publication record

34 publications (see Google Scholar, Web of Science: ABA-3331-2021, or Publication list below [1–34]) in:

Nat. Commun. (1)	J. Am. Chem. Soc. (1)	J. Chem. Theory Comput. (10)	J. Chem. Phys. (9)
Chem. Eur. J. (2)	Inorg. Chem (1)	J. Phys. Chem. A. (2)	Int. J. Quantum Chem. (2)
Theor. Chem. Acc. (2)	Phys. Status Solidi B. (1)	Chem. Phys. Lett. (1)	Mol. Phys. (2)

Publication of the year in BME and publication of the month in HAS for the co-first authored Nat. Commun. [4]
Editor's Pick [7] and Highly Cited [10] highlights in the Journal of Chemical Physics
Top 5 most read articles of the month in JCTC for 5 papers [5,6,13,14,16] (all first/last authored)
Cover pages in J. Chem. Theory Comput. [16] and J. Am. Chem. Soc. [22]

Publication list

[1] M. Kállay, R. A. Horváth, L. Gyevi-Nagy and P. R. Nagy. Basis set limit CCSD(T) energies for extended molecules via a reduced-cost explicitly correlated approach. *J. Chem. Theory Comput.* **19**, 174 (2023).

[2] A. Ott, P. R. Nagy and Z. Benkő. Stability of carbocyclic phosphinyl radicals: Effect of ring size, delocalization, and sterics. *Inorg. Chem.* **61**, 16266 (2022).

[3] P. R. Nagy, L. Gyevi-Nagy, B. D. Lőrincz and M. Kállay. Pursuing the basis set limit of CCSD(T) noncovalent interaction energies for medium-sized complexes: case study on the S66 compilation. *Mol. Phys.* **120**, e2109526 (2022).

[4] Y. S. Al-Hamdani, P. R. Nagy, D. Barton, M. Kállay, J. G. Brandenburg and A. Tkatchenko. Interactions between large molecules pose a puzzle for reference quantum mechanical methods. *Nat. Commun.* **12**, 3927 (2021).

[5] P. B. Szabó, J. Csóka, M. Kállay and P. R. Nagy. Linear-scaling open-shell MP2 approach: Algorithm, benchmarks, and large-scale applications. *J. Chem. Theory Comput.* **17**, 2886 (2021).

[6] L. Gyevi-Nagy, M. Kállay and P. R. Nagy. Accurate reduced-cost CCSD(T) energies: parallel implementation, benchmarks, and large-scale applications. *J. Chem. Theory Comput.* **17**, 860 (2021).

[7] M. Kállay, R. A. Horváth, L. Gyevi-Nagy and P. R. Nagy. Size-consistent explicitly correlated triple excitation correction. *J. Chem. Phys.* **155**, 034107 (2021).

[8] P. R. Nagy, L. Gyevi-Nagy and M. Kállay. Basis set truncation corrections for improved frozen natural orbital CCSD(T) energies. *Mol. Phys.* **119**, e1963495 (2021).

[9] S. Rahman, V. Wineman-Fisher, P. R. Nagy, Y. Al-Hamdani, A. Tkatchenko and S. Varma. Methyl-induced polarization destabilizes the noncovalent interactions of N-methylated lysines. *Chem. Eur. J.* **27**, 11005 (2021).

[10] M. Kállay, P. R. Nagy, D. Mester, Z. Rolik, G. Samu, J. Csontos, J. Csóka, P. B. Szabó, L. Gyevi-Nagy, B. Hégely, I. Ladjánszki, L. Szegedy, B. Ladóczki, K. Petrov, M. Farkas, P. D. Mezei, and Á. Ganyecz. The MRCC program system: Accurate quantum chemistry from water to proteins. *J. Chem. Phys.* **152**, 074107 (2020).

[11] V. Wineman-Fisher, J. M. Delgado, P. R. Nagy, E. Jakobsson, S. A. Pandit and S. Varma. Transferable interactions of Li^+ and Mg^{2+} ions in polarizable models. *J. Chem. Phys.* **153**, 104113 (2020).

[12] V. Wineman-Fisher, Y. Al-Hamdani, P. R. Nagy, A. Tkatchenko and S. Varma. Improved description of ligand polarization enhances transferability of ion–ligand interactions. *J. Chem. Phys.* **153**, 094115 (2020).

[13] P. R. Nagy and M. Kállay. Approaching the basis set limit of CCSD(T) energies for large molecules with local natural orbital coupled-cluster methods. *J. Chem. Theory Comput.* **15**, 5275 (2019).

[14] L. Gyevi-Nagy, M. Kállay and P. R. Nagy. Integral-direct and parallel implementation of the CCSD(T) method: Algorithmic developments and large-scale applications. *J. Chem. Theory Comput.* **16**, 366 (2020).

[15] D. Mester, P. R. Nagy and M. Kállay. Reduced-scaling correlation methods for the excited states of large molecules: Implementation and benchmarks for the second-order algebraic-diagrammatic construction approach. *J. Chem. Theory Comput.* **15**, 6111 (2019).

[16] P. R. Nagy, G. Samu and M. Kállay. Optimization of the linear-scaling local natural orbital CCSD(T) method: Improved algorithm and benchmark applications. *J. Chem. Theory Comput.* **14**, 4193 (2018).

[17] D. Mester, P. R. Nagy and M. Kállay. Reduced-cost second-order algebraic-diagrammatic construction method for excitation energies and transition moments. *J. Chem. Phys.* **148**, 094111 (2018).

[18] B. Hégely, P. R. Nagy and M. Kállay. Dual basis set approach for density functional and wave function embedding schemes. *J. Chem. Theory Comput.* **14**, 4600 (2018).

[19] Z. Szekrényes, P. R. Nagy, G. Tarczay, L. Maggini, D. Bonifazi and K. Kamarás. Direction-dependent secondary bonds and their stepwise melting in a uracil-based molecular crystal studied by infrared spectroscopy and theoretical modeling. *Chem. Phys. Lett.* **691**, 163 (2018).

[20] P. R. Nagy and M. Kállay. Optimization of the linear-scaling local natural orbital CCSD(T) method: Redundancy-free triples correction using Laplace transform. *J. Chem. Phys.* **146**, 214106 (2017).

[21] D. Mester, P. R. Nagy and M. Kállay. Reduced-cost linear-response CC2 method based on natural orbitals and natural auxiliary functions. *J. Chem. Phys.* **146**, 194102 (2017).

[22] T. Földes, Á. Madarász, Á. Révész, Z. Dobi, S. Varga, A. Hamza, P. R. Nagy, P. M. Pihko and I. Pápai. Stereocontrol in diphenylprolinol silyl ether catalyzed michael additions: Steric shielding or Curtin–Hammett scenario? *J. Am. Chem. Soc.* **139**, 17052 (2017).

[23] P. R. Nagy, G. Samu and M. Kállay. An integral-direct linear-scaling second-order Møller–Plesset approach. *J. Chem. Theory Comput.* **12**, 4897 (2016).

[24] B. Hégely, P. R. Nagy, G. G. Ferenczy and M. Kállay. Exact density functional and wave function embedding schemes based on orbital localization. *J. Chem. Phys.* **145**, 064107 (2016).

[25] P. R. Nagy, J. Koltai, P. R. Surján, Á. Szabados and J. Kürti. Resonance Raman optical activity of single walled chiral carbon nanotubes. *J. Phys. Chem. A*. **120**, 5527 (2016).

[26] V. Murg, F. Verstraete, R. Schneider, P. R. Nagy and Ö. Legeza. Tree tensor network state with variable

tensor order: an efficient multireference method for strongly correlated systems. *J. Chem. Theory Comput.* **11**, 1027 (2015).

[27] Z. Tóth, P. R. Nagy, P. Jeszenszki and Á. Szabados. Novel orthogonalization and biorthogonalization algorithms. *Theor. Chem. Acc.* **134**, 100 (2015).

[28] P. Jeszenszki, P. R. Nagy, T. Zoboki, Á. Szabados and P. R. Surján. Perspectives of APSG-based multireference perturbation theories. *Int. J. Quantum Chem.* **114**, 1048 (2014).

[29] P. R. Nagy, L. Biró, J. Koltai, P. R. Surján, Á. Szabados and J. Kürti. Theoretical vibrational optical activity of chiral carbon nanoparticles: Fullerenes and carbon nanotubes. *Phys. Status Solidi B*. **251**, 2451 (2014).

[30] P. R. Nagy, P. R. Surján and Á. Szabados. Vibrational optical activity of chiral carbon nanoclusters treated by a generalized π-electron method. *J. Chem. Phys.* **140**, 044112 (2014).

[31] P. R. Nagy and Á. Szabados. Unitary perturbation theory applied to multiconfigurational reference functions. *Int. J. Quantum Chem.* **113**, 230 (2013).

[32] P. R. Nagy, P. R. Surján and Á. Szabados. Mayer's orthogonalization: relation to the Gram–Schmidt and Löwdin's symmetrical scheme. *Theor. Chem. Acc.* **131**, 1109 (2012).

[33] G. Erős, K. Nagy, H. Mehdi, I. Pápai, P. Nagy, A. T. Rokob, K. P, G. Tárkányi and T. Soós. Catalytic hydrogenation with frustrated lewis pairs: Selectivity achieved by size-exclusion design of Lewis acids. *Chem. Eur. J.* **18**, 574 (2012).

[34] Á. Szabados and P. Nagy. Spin component scaling in multiconfiguration perturbation theory. *J. Phys. Chem. A*. **115**, 523 (2011).