Andreas Erbs Hillers-Bendtsen

Curriculum Vitae

Copenhagen, Denmark
Nationality: Danish
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Education

Feb 2021 to Apr 2024 — **Doctor of Philosophy (Ph.D.) in Theoretical and Computational Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*

- Supervisor: Professor, Ph.D., Dr. Scient. Kurt V. Mikkelsen.
- Thesis title: "Exploring Molecular Systems for Exploitation of Solar Energy Storage"

Sep 2019 to Sep 2020 — **Master of Science (M.Sc.) in Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*

- Completed in only 1 year although the standard time is 2 years with the highest possible GPA of 12/12 and a master thesis entitled "Dynamics of Photo- and Thermoinduced Reactions - Reactions of Photochromic Molecules in Environments"

Sep 2016 to Jun 2019 — **Bachelor of Science (B.Sc.) in Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*

- GPA: 12/12 and Thesis: "Quantum Classical Methods for Investigating Photochromic Molecular Systems"

Languages — Danish (native), English (fluent), and German (intermediate).

Experience

Sep 2024 to present — **Novo Nordisk Foundation Visiting Scholar** at Stanford Bio-X and Department of Chemistry, Stanford University, CA, USA

- Working as postdoctoral researcher in theoretical chemistry in the group of Professor Todd J. Martínez with funding from the Novo Nordisk Foundation.

Feb 2024 to Aug 2024 — **Postdoctoral Researcher in Theoretical Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*

Feb 2021 to Jan 2024 — **Ph.D. Fellow in Theoretical and Computational Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*

Jul 2022 to Dec 2022 — **Visiting Research Scholar**, Department of Chemistry and The Pulse Institute, Stanford University and SLAC National Accelerator Laboratory, CA, USA.

- A research stay in the group of Professor Todd J. Martínez during my Ph.D. studies.

Oct 2020 to Jan 2021 — **Scientific Assistant**, *Department of Chemistry, University of Copenhagen, DK.*

- Research concerning how to investigate and design molecular systems that can capture, store, and exploit solar radiation with Professor, Ph.D., Dr. Scient. Kurt V. Mikkelsen.

Aug 2018 — **Instructor**, *Department of Chemistry, University of Copenhagen, DK.*

to Sep 2020
- Teaching assistant in the 1st year B.Sc. course "Chemical Bonding" in the spring semester 2020.
- Teaching assistant in the 1st year B.Sc. course "Introduction to the Mathematics for the Chemical Sciences" in the fall semester 2019.

Dec 2017 **Student Assistant**, *Novozymes, DK*

to Aug 2020
- Assisting in general laboratory work including preparation of eluents, buffers, and other solutions relevant for current tests running, cleaning in the lab, and ordering required equipment and miscellaneous items. Additionally, assisting in registering samples, enzymes, chemicals, and results of analysis in the database.

Awards, Grants and Scholarships

2024-2028 **Novo Nordisk Foundation Stanford Bio-X Postdoctoral Fellowship** (3.309.175 DKK ≈ 475.000 USD) from the Novo Nordisk Foundation for a three-year stay with Professor Todd J. Martínez at Stanford University and subsequent return to University of Copenhagen.

2024 **Award: Ph.D. Prize 2024 at the Faculty of Science, University of Copenhagen** awarded to the three best Ph.D. theses.

2023 **Co-PI on U.S. Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment**: A software development project with a computer time allocation granting a total of 300000 node hours on the Frontier computing cluster at the Oak Ridge Leadership Computing Facility, Oak Ridge National Laboratory, TN, USA.

2021 **Elite Researcher Ph.D. travel grant** (200.000 DKK ≈ 30.000 USD) from The Danish Council for Independent Research and the Ministry of Higher Education and Research, Denmark

2020 **Award: Master thesis of the year 2020** at Department of Chemistry, University of Copenhagen

Talks and Presentations

Aug 2024 Invited talk at the Annual Meeting of the Danish Chemical Society 2024, Lyngby, Denmark: "Probing the Ultrafast Photodynamics of Dihydroazulene Derivatives using Quantum Chemistry"

Aug 2024 Contributed talk at the Scandinavian Community for Quantum Chemistry meeting 2024, Odense, Denmark: "Cluster perturbation theory: perturbation series for coupled cluster singles doubles ground state energies

Jun 2024 Poster at the European Seminar on Computational Methods in Quantum Chemistry 2024, Copenhagen, Denmark: "Cost Effective Large Scale Third Order Excitation Energies through Cluster Perturbation Theory on Graphical Processing Units"

Aug 2023 Poster at the Annual Meeting of the Danish Chemical Society 2023, Copenhagen, Denmark: "Probing the Ultrafast Photodynamics of Dihydroazulene with In Silico Time Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction"

Jun 2023 Poster at the International Congress of Quantum Chemistry 2023, Batislava, Slovakia: "Probing the Ultrafast Photodynamics of Dihydroazulene with In Silico Time Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction"

Jun 2023 Seminar at the Advanced Computing for Chemistry & Materials Group, National Center for Computational Sciences Division, Oak Ridge National Laboratory, TN, USA: "Massively Parallel GPU Enabled Third-order Cluster Perturbation Excitation Energies for Cost-effective Large Scale Excitation Energy Calculations"

Jun 2022 Talk at the MOST - Molecular Solar Thermal Energy Storage Systems EU Project Conference, Gothenburg, Sweden: "Computational Design of Bicyclic Dienes for Solar Energy Storage"

Nov 2021 Seminar at the Department of Theoretical Chemistry and Biology, KTH Royal Institute of Technology, Stockholm, Sweden: "Cluster Perturbation Theory: Perturbation Series for CCSD Energies"

Apr 2021 Seminar in the Center for Exploitation of Solar Energy, Department of Chemistry, University of Copenhagen: "Can we use $[2,2,2]$-bicyclooctadienes for storing solar energy?"

Apr 2021 Seminar for Theoretical Chemistry, Department of Chemistry, University of Copenhagen:"Cluster perturbation theory: Fast results of CCSD quality"

Dec 2019 Seminar in the Center for Exploitation of Solar Energy, Department of Chemistry, University of Copenhagen: "RRKM rate constants of the photoisomerization of dihydroazulene and aromatic derivatives "

Oct 2019 Seminar in the Center for Exploitation of Solar Energy, Department of Chemistry, University of Copenhagen:"Tuning the properties of dihydroazulene/vinylheptafulvene with nanoparticles"

Nov 2018 Seminar in the Center for Exploitation of Solar Energy, Department of Chemistry, University of Copenhagen: "Investigating the properties of dihydroazulene/vinylheptafulvene under influence of nanoparticles"

Software Developments

Penguin: A Python Module for Electronic Structure Calculations using Coupled Cluster Theory, Møller-Plesset Perturbation Theory, and Cluster Perturbation Theory.

- Lead Developer and Founder of the program with contributions to all aspects of the code.

LSDalton: An Electronic Structure Program for Linear Scaling Hartree-Fock and Density Functional Theory as well as Coupled Cluster Theory.

- Developer of the Cluster Perturbation Theory module which enables massively parallel and GPU-accelerated molecular property calculations.

Dalton: An All-Purpose Electronic Structure Program for Molecular Property Calculations.

- Implemented MP3 wave functions and energies which are also used in the TOPPA module.

List of Publications

39. A. S. Aslam, L. M. Muhammad, A. E. Hillers-Bendtsen, K. V. Mikkelsen, K. Moth-Poulsen, "Norbornadiene-Quadricyclane photoswitches with enhanced solar spectrum match", Chem. Eur. J., 30, 46, e202401430, 2024

38. S. Ghasemi, M. Shamsabadi, A. Olesund, A. E. Hillers-Bendtsen, F. Najera, F. Edhborg, A. S. Aslam, W. Larsson, Z. Wang, F. M. A. Noa, R. J. Salthouse, L. Öhrström, H. Hölzel, E. Perez-Inestrosa, K. V. Mikkelsen, J. Hanrieder, B. Albinsson, A. Dreos, K. Moth-Poulsen: "Pyrene functionalized norbornadiene-quadricyclane fluorescent photoswitches: characterization of their spectral properties and application in imaging of amyloid beta plaques", Chem. Eur. J., 30, 34, e202400322, 2024

37. P. Jørgensen, J. Olsen, M. B. Johansen, T. J. von Buchwald A. E. Hillers-Bendtsen, K. V. Mikkelsen, T. Helgaker: "A Variational Reformulation of Molecular Properties in Electronic-Structure Theory", Sci. Adv., 10, 17, eadn3454, 2024

36. A. E. Hillers-Bendtsen, Y. Todarwal, P. Norman and K. V. Mikkelsen, "Dynamical Effects of Solvation on Norbornadiene/Quadricyclane Systems", J. Phys. Chem. A, 128, 13, 2602–2610, 2024

35. A. E. Hillers-Bendtsen, F. Jensen, K. V. Mikkelsen, J. Olsen, and P. Jørgensen, "Cluster perturbation theory IX: Perturbation series for the coupled cluster singles and doubles ground-state energy", J. Chem. Phys., 160, 104108, 2024

34. A. E. Hillers-Bendtsen, K. V. Mikkelsen, and T. J. Martínez, "Tensor Hypercontraction of Cluster Perturbation Theory: Quartic Scaling Perturbation Series for the Coupled Cluster Singles and Doubles Ground State Energies", J. Chem. Theo. Comput., 20, 5, 1932–1943, 2024

33. A. E. Hillers-Bendtsen, Y. Zhou, K. V. Mikkelsen, "Investigation of Solvent Effects on Molecular Energy Storage and Optical Properties of Bicycloctadiene/ Tetracyclooctane Photoswitches", J. Phys. Chem. A, 128, 1, 41-50, 2024

32. J. Granhøj, M. Zalibera, M. Malček, V. B. R. Pedersen, A. E. Hillers-Bendtsen, K. V. Mikkelsen, P. Rapta and M. B. Nielsen, "Extended Tetrathiafulvalenes with Fluoreno[3,2-b]fluorene and Diindeno[1,2-b:1',2'-i]anthracene Cores", Chem. Eur. J., 30, 5, e202302688, 2024

31. F. Ø. Kjeldal, A. E. Hillers-Bendtsen, K. V. Mikkelsen, "The influence of silver and copper nanoparticles on the optical properties of photochromic molecules", Nanosci. Nanotechnol. Open Access, 2(2), 1018, 2023

30. S. Ghasemia, L. Ornago, Z. Liasi, M. B. Johansen, T. J. von Buchwald, A. E. Hillers-Bendtsen, S. van der Poel, H. Hölzel, Z. Wang, F. M. A. Noa, L. Öhrström, K. V. Mikkelsen, H. Van Der Zant, S. Lara-Avil, and K. Moth-Poulsen, "Exploring the impact of select anchor groups for norbornadiene/quadricyclane single-molecule electronic switches", J. Mater. Chem. C, 11, 15412-15418, 2023

29. S. S. Warthegau, A. E. Hillers-Bendtsen, S. K. Pedersen, C. Rindom, C. Bræstrup, J. S. Jensen, O. Hammerich, M. S. Thomsen, F. S. Kamounah, P. Norman, K. V. Mikkelsen, T. Brock-Nannestad, M. Pittelkow, "Heterocyclic [9]helicenes exhibiting bright circular polarized luminescence", Chem. Eur. J., 29, 58, e20230181, 2023

28. A. E. Hillers-Bendtsen, J. L. Elholm, O. B. Obel, H. Hölzel, K. Moth-Poulsen, and K. V. Mikkelsen, "Searching the Chemical Space of Bicyclic Dienes for Molecular Solar Thermal Energy Storage Candidates", Angew. Chem. Int. Ed., 62, 40, e2023095, 2023

27. I. L. H. Kjeldsen, J. F. Høvring, A. E. Hillers-Bendtsen, and K. V. Mikkelsen, "The Effects of Solvent Dynamics on the Back Reaction of Solar Thermal Energy Storage Systems", J. Phys. Chem. A, 127, 34, 7058–7069, 2023

26. M. D. Jensen, C. T. Hansen, A. E. Hillers-Bendtsen, and K. V. Mikkelsen, "Investigation of Coulomb Blockade Diamonds of 7-Helicene Interacting with Gold Nanoparticles", Chem. Phys. Lett., 830, 140761, 2023

25. J. L. Elholm, Z. Liasi, M. K. Mikkelsen, A. E. Hillers-Bendtsen, and K. V. Mikkelsen, "Computational Investigation of Photoswitch Conjugates for Molecular Solar Energy Storage", Phys. Chem. Chem. Phys., 25, 21964-21969, 2023

24. Z. Liasi, A. E. Hillers-Bendtsen, L. Jensen, K. V. Mikkelsen, "Elucidating the mystery of DNA-templating effects on a silver nanocluster", J. Phys. Chem. Lett., 14, 25, 5727–5733, 2023

23. H. H. Corzo, A. E. Hillers-Bendtsen, A. L. Barnes, A. Y. Zamani, F. Pawlowski, J. Olsen, P. Jørgensen, K. V. Mikkelsen, and D. Bykov, "Coupled Cluster Theory on Modern Heterogeneous Supercomputers", Front. Chem., 11, 321, 2023

22. A. E. Hillers-Bendtsen, D. Bykov, A. L. Barnes, D. Liakh, H. H. Corzo, J. Olsen, P. Jørgensen, and K. V. Mikkelsen, "Massively Parallel GPU Enabled Third Order Cluster Perturbation Excitation Energies for Cost-Effective Large Scale Excitation Energy Calculations", J. Chem. Phys., 158, 144111, 2023

21. J. S. Rodrigo, A. E. Hillers-Bendtsen, F. Ø. Kjeldal, N. M. Høyer, K. V. Mikkelsen, and S. P. A. Sauer, "Indirect nuclear spin-spin couplings with third order contributions added to the SOPPA method", J. Chem. Phys., 158, 124118, 2023

20. J. L. Elholm, A. E. Hillers-Bendtsen, H. Hölzel, K, Moth-Poulsen, and K. V. Mikkelsen, "High Throughput Screening of Norbornadiene/Quadricyclane Derivates for Molecular Solar Thermal Energy Storage", Phys. Chem. Chem. Phys., 24.47, 28956-28964, 2022

19. A. E. Hillers-Bendtsen, F. Ø. Kjeldal, N. Ree, E. Matito, and K. V. Mikkelsen, "Excited State Dynamics and Conjugation Effects of the Photoisomerization Reactions of Dihydroazulene", Phys. Chem. Chem. Phys., 24.47, 28934-28943, 2022

18. A. E. Hillers-Bendtsen, Y. Todarwal, M. Pittelkow, P. Norman and K. V. Mikkelsen, "Modelling absorption and emission spectroscopies of symmetric and asymmetric azaoxahelicenes in vacuum and solution", J. Phys. Chem. A, 126, 37, 6467-6472, 2022

17. A. E. Hillers-Bendtsen, N. M. Høyer, F. Ø. Kjeldal, K. V. Mikkelsen, J. Olsen, and P. Jørgensen, "Cluster perturbation theory VIII: First order properties for a coupled cluster state", J. Chem. Phys., 157, 024107, 2022

16. J. Olsen, A. E. Hillers-Bendtsen, N. M. Høyer, F. Ø. Kjeldal, K. V. Mikkelsen, and P. Jørgensen, "Cluster perturbation theory VII: The convergence of cluster perturbation expansions", J. Chem. Phys., 157, 024106, 2022

15. N. M. Høyer, F. Ø. Kjeldal, A. E. Hillers-Bendtsen, K. V. Mikkelsen, J. Olsen, and P. Jørgensen, "Cluster perturbation theory. VI. Ground-state energy series using the Lagrangian", J. Chem. Phys., 157, 024105, 2022

14. A. E. Hillers-Bendtsen, F. Ø. Kjeldal, and K. V. Mikkelsen, "Electric properties of photochromic molecules physisorbed on silver and copper nanoparticles", J. Phys. Chem A., 126, 20, 3145–3156, 2022

13. A. E. Hillers-Bendtsen, P. G. I. L. Dünweber, L. H. Olsen and K. V. Mikkelsen, "Prospects of Improving Molecular Solar Energy Storage of the Norbornadiene/Quadricyclane System through Bridgehead Modifications", J. Phys. Chem. A, 126, 17, 2670–2676, 2022

12. D. N. Essenbæk, A. E. Hillers-Bendtsen, and K. V. Mikkelsen, "Linear optical absorptions of photo/thermochromic organic molecules interacting with a gold nanoparticle", Asian J. Appl. Chem. Res., 11(1), 1-16, 2022

11. I. L. H. Kjeldsen, J. F. Høvring, T. J. von Buchwald, A. E. Hillers-Bendtsen, and K. V. Mikkelsen, "On the Effects of Solvation on the Back Reaction and Storage Capabilities of Solar Thermal Energy Storage Systems", Phys. Chem. Chem. Phys., 24, 5564–5577, 2022

10. A. E. Hillers-Bendtsen, F. Ø. Kjeldal, N. M. Høyer, and K. V. Mikkelsen, "Optimization of the thermochemical properties of the Norbornadiene/ Quadricyclane photochromic couple for solar energy storage using nanoparticles", Phys. Chem. Chem. Phys., 24, 5506–5521, 2022

9. M. Quant, A. E. Hillers-Bendtsen, S. Ghasemi, M. Erdelyi, Z. Wang, L. M. Muhammad, N. Kann, K. V. Mikkelsen, and K. Moth-Poulsen , "Synthesis, Characterization and Computational Evaluation of Bicyclooctadienes for Molecular Solar Thermal Energy Storage", Chem. Sci., 13, 834-841, 2022

8. A. E. Hillers-Bendtsen, M. Quant, K. Moth-Poulsen, and K. V. Mikkelsen, "A Benchmark investigation of the structural and thermochemical properties of a series of [2.2.2]-Bicyclooctadienes photoswitches", J. Phys. Chem. A, 125, 48, 10330–10339, 2021

7. A. Mengots, A. E. Hillers-Bendtsen, S. Doria, F. Ø. Kjeldal, N. M. Høyer, A. U. Petersen, K. V. Mikkelsen, M. Di Donato, M. Cacciarini, and M. B. Nielsen, "Dihydroazulene-azobenzene-dihydroazulene triad photoswitches", Chem. Eur. J., 27, 12437-12446, 2021

6. A. E. Hillers-Bendtsen, M. B. Johansen, and K. V. Mikkelsen, "Promoting the thermal back reaction of Vinylheptafulvene to Dihydroazulene by physisorbtion on metallic nanoparticles", Phys. Chem. Chem. Phys., 23, 12889-12899, 2021

5. V. B. R. Pedersen, J. Granhøj, A. E. Hillers-Bendtsen, A. Kadziola, K. V. Mikkelsen, and M. B. Nielsen, "Fulvalene-Based Polycyclic Aromatic Hydrocarbon Ladder-type Structures – Synthesis and Properties", Chem. Eur. J., 27, 8315–8324, 2021

4. A. E. Hillers-Bendtsen, M. B. Johansen, and K. V. Mikkelsen, "Teoria do estado de transição: Dihydroazulene/Vinylheptafulvene", Book Chapter in A Química nas Áreas Natural, Tecnológica e Sustentável, 3, 388-416, 2020

3. A. E. Hillers-Bendtsen, F. Ø. Kjeldal, and K. V. Mikkelsen, "Molecular solar thermal energy storage properties of photochromic molecules physisorbed onto nanoparticles" Chem. Phys. Lett., 733, 136661, 2019

2. A. E. Hillers-Bendtsen and K. V. Mikkelsen, "The influence of gold nanoparticles on the two photon absorption of photochromic molecular systems" Phys. Chem. Chem. Phys., 21, 18577-18588, 2019

1. A. E. Hillers-Bendtsen, M. H. Hansen, and K. V. Mikkelsen, "The influence of nanoparticles on the excitation energies of the photochromic dihydroazulene/vinylheptafulvene system" Phys. Chem. Chem. Phys., 21, 6689-6698, 2019