

# Andreas Erbs Hillers-Bendtsen

## Curriculum Vitae

+4551161524

✉ aehb@chem.ku.dk

Nationality: Danish

Date of birth: 28-12-1996

### Scientific area

Physical Chemistry, Theoretical Chemistry, Computational Chemistry

### Working experience

- Jul 2022 **Visiting Research Scholar**, Department of Chemistry and Pulse Institute, Stanford University and SLAC National Accelerator Laboratory, CA, USA.
- to Present A five month research stay in the group of Professor Todd J. Martínez during my Ph.D. studies working on simulations of photochemical and photophysical processes in solar energy storage systems from first principles as well as tensor hypercontraction of Cluster Perturbation theory.
- Feb 2021 **Ph.D. Fellow in Theoretical and Computational Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*
- to Present
- The Ph.D. project concerns how to investigate and design molecular systems that can capture, store, and exploit solar radiation as well as development and implementation of advanced molecular electronic structure models using Cluster Perturbation theory. The project has the working title: "Exploring Molecular Systems for Exploitation of Solar Energy & Development of Cluster Perturbation Theory" and is carried out under supervision of Professor, Ph.D., Dr. Scient. Kurt V. Mikkelsen.
  - **Expected end date of the Ph.D. project:** 28.02.2024
- Oct 2020 **Scientific Assistant**, *Department of Chemistry, University of Copenhagen, DK.*
- Jan 2021
- Working on a research project that concerned how to investigate and design molecular systems that can capture, store, and exploit solar radiation in the group of Professor, Ph.D., Dr. Scient. Kurt V. Mikkelsen.
- Aug 2018 **Instructor**, *Department of Chemistry, University of Copenhagen, DK.*
- 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*

- 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.

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## Education

- Feb 2021 **Doctor of Philosophy (Ph.D.) in Theoretical and Computational Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*
- to Present ○ **Expected end date of the Ph.D. project:** 28.02.2024
- Sep 2019 **Master of Science (MSc) in Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*
- to Sep 2020 ○ Completed 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 **Bachelor of Science (BSc) in Chemistry**, *Department of Chemistry, University of Copenhagen, DK.*
- to Jun 2019 ○ Completed with the highest possible GPA of 12/12 and a bachelor thesis entitled "Quantum Classical Methods for Investigating Photochromic Molecular Systems"
- 2009–2013 **Advanced secondary education**, *Skanderborg Gymnasium, Advanced secondary education institution, DK.*
- Graduated, with a GPA of 11.9/12 excluding bonuses. Weighted GPA of 12.3/12 including 3 % bonus for an additional A-level course.
  - A levels: Chemistry, Mathematics, English, History, Danish.
- Languages Danish (native), English (fluent), and German (intermediate).

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## Awards, Grants and Scholarships

- 2021 **Elite Researcher Ph.D. travel grant** (200 thousand DKK) 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
- 2019 **Travel grant** (4000 DKK) from The Danish Chemical Society

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## Other activities

- June 2018 **Chairman of the organisation for Chemistry students 'Kemisk Fagråd' at the University of Copenhagen.**
- June 2020
- Feb 2017 **Member of the study board for chemistry, physics, and nanoscience**, *Faculty of Science, University of Copenhagen, DK.*

- Sep 2020 ○ As Vice Chairman from Feb 2018 - Sep 2020 playing an active role planning and altering the structure of the educations offered at the Department of Chemistry, University of Copenhagen.

## Talks and presentations

- 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"
- Apr 2022 Online seminar in the group of Professor Todd J. Martínez, Department of Chemistry, Stanford University, California, USA: "Exploitation of Solar Energy and Cluster Perturbation Theory"
- 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"

## List of publications

- F. Ø. Kjeldal, A. E. Hillers-Bendtsen, N. M. Høyer, K. V. Mikkelsen, J. Olsen, and P. Jørgensen, "Cluster perturbation theory IX: Perturbation series for the coupled cluster singles and doubles ground-state energy", In Preparation.
- J. L. Elholm, M. K. Mikkelsen, A. E. Hillers-Bendtsen, and K. V. Mikkelsen, "Computational Investigation of Photoswitch Conjugates for Molecular Solar Energy Storage", Submitted to Phys. Chem. Chem. Phys.
- 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", Submitted to Phys. Chem. Chem. Phys.
- A. E. Hillers-Bendtsen, F. Ø. Kjeldal, N. Ree, Eduard Matito, and K. V. Mikkelsen, "Excited State Dynamics and Conjugation Effects of the Photoisomerization Reactions of Dihydroazulene", Submitted to Phys. Chem. Chem. Phys.
- 2022 A. E. Hillers-Bendtsen, Y. Tadarwal, M. Pittelkow, P. Norman and K. V. Mikkelsen, "Modelling absorption and emission spectroscopies of symmetric and asymmetric azaoxahelicenes in vacuum and solution", Accepted for Publication in J. Phys. Chem. A
- 2022 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, DOI:10.1063/5.0082585
- 2022 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, DOI:10.1063/5.0082584
- 2022 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, DOI:10.1063/5.0082583
- 2022 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, DOI:10.1021/acs.jpca.2c01003
- 2022 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, DOI: 10.1021/acs.jpca.2c00950
- 2022 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. DOI: 10.9734/ajacr/2022/v11i130243
- 2022 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, DOI: 10.1039/D2CP00401A
- 2022 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, DOI: 10.1039/D2CP00226D

- 2022 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, DOI: 10.1039/D1SC05791J
- 2021 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, DOI: 10.1021/acs.jpca.1c07737
- 2021 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, DOI: 10.1002/chem.202101533
- 2021 A. E. Hillers-Bendtsen, M. B. Johansen, and K. V. Mikkelsen, "Promoting the thermal back reaction of Vinylheptafulvene to Dihydroazulene by physisorption on metallic nanoparticles", *Phys. Chem. Chem. Phys.*, 23, 12889-12899, 2021, DOI: 10.1039/D0CP02893B
- 2021 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, DOI: 10.1002/chem.202100984
- 2020 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
- 2019 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, DOI: 10.1016/j.cplett.2019.136661
- 2019 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, DOI: 10.1039/C9CP03283E
- 2019 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, DOI: 10.1039/C8CP06539J