

Klaus Braagaard Møller, Professor



Education

- DTU Leadership Programme, 2012
- Ph.D. in Chemistry, DTU, 1997
- M.Sc. in Engineering, DTU, 1993

Employment

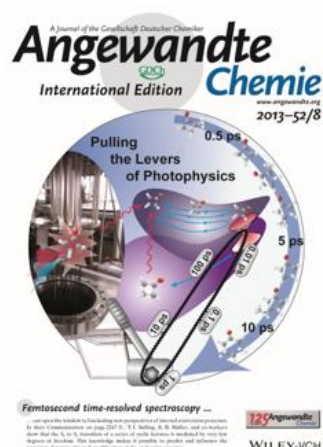
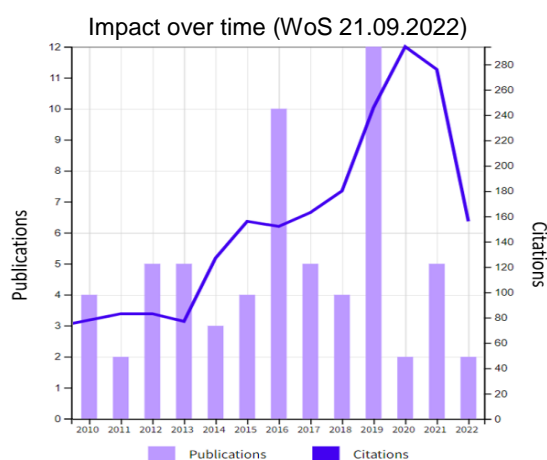
- Professor, Department of Chemistry, DTU, 2016-
- Head of Section, Physical and Biophysical Chemistry, Department of Chemistry, DTU, 2015-
- Head of studies, B.Sc. program "Chemistry & Technology", DTU, 2010-
- Associate professor, Department of Chemistry, DTU, 2005-2016
- Assistant professor, Department of Chemistry, DTU, 2002-2005
- Young Researcher (w. J.T. Hynes), Département de Chimie, ENS Paris, France, 2001-2002
- Postdoctoral Scholar (w. A.H. Zewail), Division of Chemistry, Caltech, USA, 1997-2001
- Visiting Scientist, Center for Research and Advanced Studies, IPN, Mexico, 1997
- Research assistant (w. E.J. Heller), Department of Physics, Harvard University, USA, 1994-95

Research management

- Guest editor, *Structural Dynamics*, 2021
- Co-organizer, 13th Nordic Femtochemistry Meeting, Denmark, 2018
- Member of management committee, COST action CM1405 MOLIM, 2014-2019
- Local Scientific Organizer, 11th International Femtochemistry Conference, Denmark, 2013
- Co-organizer, 8th Nordic Femtochemistry Meeting, Denmark, 2008
- Co-founder of Danish National Research Foundation Center for Molecular Movies, 2005-2013

Publications

- Peer-reviewed publications: 95 research papers, 2 book chapters, and 6 proceedings
- Average citations per publication: 26.4 (WoS 21.09.2022)
- H-Index: 29 (WoS 21.09.2022), 33 (Google Scholar 21.09.2022)
- Articles in high-profile journals since 2010: *Nat. Commun.* (4), *Angew. Chem. Int. Ed.* (2), *Chem. Sci.* (1), *J. Am. Chem. Soc.* (3), *Phys. Rev. Lett.* (3), *J. Phys. Chem. Lett.* (3)



[Homepage](#), [Google Scholar](#), [ORCID](#), [ResearcherID](#), [ResearchGate](#)

Other scientific activities

- Serves as referee for numerous scientific journals
- Given more than 30 invited talks at international conferences, including (3 cancelled in 2020)
 - CECAM: Nonequilibrium solvent effects on excited states, France (online), 14-17/6, 2021
 - 14th International Femtochemistry Conference, China, 28/7-2/8, 2019
 - CECAM: Theoretical and Computational Inorganic Photochemistry, France, 17-20/6, 2019
 - 10th International Meeting on Photodynamics and Related Aspects, Colombia, 3-7/9, 2018
 - International Workshop on Molecular Quantum Dynamics, Switzerland, 18-20/4, 2017

Supervision of PhD students and postdocs

- Currently supervisor of 3 PhD students
- Successfully completed supervision of 14 PhD students and 6 postdocs
- Prizes obtained by my PhD students:
 - Springer Ph.D. thesis award “Best of the Best”, 2012, 2013, 2015, 2019
 - Danish Ministry of Education EliteForsk travel grant, 2010, 2015
 - Danish Chemical Society Ph.D. thesis award in molecular spectroscopy, 2015
 - Danish Chemical Society Ph.D. thesis award in organic chemistry, 2013
 - DTU’s Young Researcher Award, 2013

Recent external funding

- Independent Research Fund Denmark, 6.2 MDKK, co-PI (50%), 2022-2026
- Independent Research Fund Denmark, 5.9 MDKK, co-PI (50%), 2018-2022
- European Commission H2020-MSCA-ITN, 3.7 M€, co-applicant, 2018-2022
- Danish Council for Independent Research: 6.5 MDKK, co-PI (50%), 2014-2019
- Lundbeck Foundation: 1 MDKR, main applicant, 2011-2013
- Danish National Research Foundation: 35 MDKK, co-applicant, 2005-2013

Recent scientific highlights

- I developed new computational strategies for inter- and intramolecular energy transfer in organic photochemistry (Angew. Chem. 2013, JPCL 2019, PCCP 2021, Nat. Commun. 2021, JPPA 2022) and in functional molecules for photo-catalysis (JPCL 2014, JPCC 2018) and light-harvesting (JPCC 2016, 2019, JACS 2022).
- I pioneered first-principles theory of ultrafast X-ray scattering and spectroscopy on the femtosecond (JPCB 2008, JCP 2019) and attosecond (PCCP 2017, PRL 2019) timescales.
- In collaborations with experimental groups from all over the world, I headed the theoretical and computational contributions to the interpretations of ground-breaking ultrafast X-ray scattering experiments in solution, visualizing for the first time: geminate reformation of molecules (JACS 2013), vibrations in molecules (PRL 2016, 2019), active-site dynamics of a photocatalyst (Nat. Commun. 2016), and energy flow in light-harvesters (Chem. Sci. 2019, Angew. Chem. 2020, Nat. Commun. 2020).

Teaching and outreach activities

- Course responsible/teacher of more than 10 different courses at all university levels, 2005-
- Member of Study Board (Chairman 2012-2015), Department of Chemistry, DTU, 2009-
- Member of many committees concerning education and teaching, DTU, 2010-
- Regularly giving talks on science and education to high-school students, 2010-
- Recipient of the Teacher of the Year award, DTU, 2008
- Appearances on TV: [Academy of the Danes](#) (DR2, 2010), [Murder in Movies](#) (DR3, 2015)