Jacob Kongsted
Department of Physics, Chemistry and Pharmacy
Chemistry and Pharmacy
Email: kongsted@sdu.dk
Phone: +4565502304

Publications

Reduced Density Matrix Formulation of Quantum Linear Response
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NMR spin-spin coupling constants in polymethine dyes as polarity indicators
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On the importance of excited state dynamic response electron correlation in polarizable embedding methods
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Parallelization of the polarizable embedding scheme for higher-order response functions
Steindal, A. H., Olsen, J. M. H., Frediani, L., Kongsted, J. & Ruud, K., 2012, In: Molecular Physics. 110, 19-20, p. 2579-2586

Performance of popular XC-functionals for the description of excitation energies in GFP-like chromophore models
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PERI-CC2: a polarizable embedded RI-CC2 method
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Quantification of the pi-pi Interactions that Govern Tertiary Structure in Donor–Acceptor [2]Pseudorotaxanes
Hansen, S. W., Stein, P. C., Sørensen, A., Share, A. I., Witlicki, E. H., Kongsted, J., Flood, A. H. & Jeppesen, J. O., 2012, In: Journal of the American Chemical Society. 134, 8, p. 3857-3863

The role of molecular conformation and polarizable embedding for one- and two-photon absorption of disperse orange 3 in solution
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Accurate Predictions of Nonpolar Solvation Free Energies Require Explicit Consideration of Binding-Site Hydration
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A Theoretical Investigation of Gas Phase NO3 Initiated Nitration of p-Cresol
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Kjær, H., P.A. Sauer, S., Kongsted, J., Yu, Y. & Krivdin, L. B., 2011, In: Chemical Physics. 381, p. 35

Benchmarking the multipole shielding polarizability/reaction field approach to solvation against QM/MM: Applications to the shielding constants of N-methylacetamide
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Computational Protocols for Prediction of Solute NMR Relative Chemical Shifts: A Case Study of L-Tryptophan in Aqueous Solution
Eriksen, J. J., Olsen, J. M. H., Aidas, K., Ågren, H., Mikkelsen, K. V. & Kongsted, J., 2011, In: Journal of Computational Chemistry. 32, 13, p. 2853-2864

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Demystifying the solvatochromic reversal in Brooker´s merocyanine dye
Murugan, N. A., Kongsted, J., Rinkevicius, Z. & Ågren, H., 2011, In: Physical Chemistry Chemical Physics. 13, 4, p. 1290-1292

Density Functional Theory/Molecular Mechanics Approach for Electronic g-Tensors of Solvated Molecules
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Excitation energies in solution: the full polarizable QM/MM/PCM method
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Fluorescence and phosphorescence of acetone in neat liquid and aqueous solution studied by QM/MM and PCM approaches
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Hybrid density functional theory / molecular mechanics calculations of two-photon absorption of dimethyl-amino-nitro-stilbene in solution
Murugan, N. A., Kongsted, J., Rinkevicius, Z., Aidas, K., Mikkelsen, K. V. & Ågren, H., 2011, In: Physical Chemistry Chemical Physics. 13, p. 12506

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Molecular Properties through Polarizable Embedding
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Optimized Basis Sets for Calculation of Electron Paramagnetic Resonance Hyperfine Coupling Constants: aug-cc-pVTZ-J for the 3d Atoms Sc–Zn
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Photosynthetic Light-Harvesting Is Tuned by the Heterogeneous Polarizable Environment of the Protein
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Solvation Effects on Electronic Transitions: Exploring the Performance of Advanced Solvent Potentials in Polarizable Embedding Calculations
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Solvatochromic shifts versus nanosolvation patterns: uracil in water as a test case
Zazza, C., Olsen, J. M. & Kongsted, J., 2011, In: Computational and Theoretical Chemistry. 974, 1-3, p. 109-116

The coupling constant polarizability and hyperpolarizabilty of 1J(NH) in N-methylacetamide, and its application for the multipole spin–spin coupling constant polarizability/reaction field approach to solvation
Kjær, H., Sauer, S. P. A. & Kongsted, J., 2011, In: Journal of Computational Chemistry. 32, p. 3168-3174

The polarizable embedding coupled cluster method
Sneskov, K., Schwabe, T., Kongsted, J. & Christiansen, O., 2011, In: The Journal of Chemical Physics. 134, p. 104-108

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Approximate inclusion of triples excitations in combined coupled cluster/molecular mechanics: Calculations of electronic excitation energies in solution for acrolein, water, formamide, and N-methylacetamide
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Kjær, H., Sauer, S. P. A. & Kongsted, J., 2010, In: The Journal of Chemical Physics. 133, p. 144160

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Interpretation of the ultrafast photo-induced processes in pentacene thin films
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Ligand affinities estimated by quantum chemical calculations
Soderhjelm, P., Kongsted, J. & Ryde, U., 2010, In: Journal of Chemical Theory and Computation. 6, p. 1726

Modeling absorption spectra of stilbazolium merocyanine in water using hybrid QM/MM techniques
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Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques
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Nonlinear optical effects induced by nano particles in symmetric molecules
Hansen, T., Hansen, T., Mikkelsen, K. V., Kongsted, J. & Mujica, V., 2010, In: Journal of Physical Chemistry C. 114, p. 20870

Non-polar solvation free energies of protein-ligand complexes
Genheden, S., Kongsted, J., Soderhjelm, P. & Ryde, U., 2010, In: Journal of Chemical Theory and Computation. 6, p. 3558

On the existence of the H3 tautomer of adenine in aqueous solution. Rationalizations based on hybrid quantum mechanics/molecular mechanics predictions
Aidas, K., Mikkelsen, K. V. & Kongsted, J., 2010, In: Physical Chemistry Chemical Physics. 12, p. 761

Solvatochromic Shifts in Uracil: A Combined MD-QM/MM Study
Olsen, J. M., Aidas, K., Mikkelsen, K. V. & Kongsted, J., 2010, In: Journal of Chemical Theory and Computation. 6, p. 249

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Kongsted, J. & Ryde, U., 2009, In: Journal of Computer - Aided Molecular Design. 23, p. 63

Charge transfer excitation energies in pyridine-silver complexes: a QM/MM investigation.
Vaida, A., Kongsted, J., Mikkelsen, K. V. & Hansen, T., 2009, In: Chemical Physics Letters. 470, p. 285

Electronic energy transfer in condensed phase studied by a polarizable QM/MM model
Curutchet, C., Munoz-Losa, A., Monti, S., Kongsted, J., Scholes, G. D. & Mennucci, B., 2009, In: Journal of Chemical Theory and Computation. 5, p. 1838

How accurate are continuum solvation models for drug-like molecules?
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On the importance of vibrational contributions to small-angle optical rotation: Fluoro-oxirane in gas phase and solution
Pedersen, T. B., Kongsted, J., Crawford, T. D. & Ruud, K., 2009, In: The Journal of Chemical Physics. 130, p. 034310

Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics
Møgelhøj, A., Kestutis, A., Mikkelsen, K. V., Sauer, S. P. A. & Kongsted, J., 2009, In: The Journal of Chemical Physics. 130, p. 134508

Vibrationally averaged optical rotations from combined coupled clusterand density functional theory
Pedersen, T. B., Kongsted, J. & Crawford, T. D., 2009, In: Chirality. 21, p. S68

Activities

Advances in Quantum Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2012

Beregningsmetoder til at forstå molekylstruktur og dynamik
Kongsted, J. (Lecturer)
3. Nov 2010

Censor på Bachelorprojekt KIKU (External organisation)
Kongsted, J. (Chairman)
24. Jun 2011

Censor på PhD kursus
Kongsted, J. (Censor)
19. Oct 2011

Chemical Physics Letters (Journal)
Kongsted, J. (Editor)
1. Jan 2010

Chemical Physics Letters (Journal)
Kongsted, J. (Peer reviewer)
7. Sept 2010 → …

Chemical Physics Letters (Journal)
Kongsted, J. (Peer reviewer)
2010

Chemical Physics Letters (Journal)
Kongsted, J. (Peer reviewer)
2011

Chemical Physics Letters (Journal)
Kongsted, J. (Peer reviewer)
2011

Chemical Physics Letters (Journal)
Kongsted, J. (Peer reviewer)
2011

Chemical Physics Letters (Journal)
Kongsted, J. (Peer reviewer)
2011

Chemistry - A European Journal (Journal)
Bähring, S. (Peer reviewer), Olsen, G. (Peer reviewer), Stein, P. C. (Peer reviewer), Kongsted, J. (Peer reviewer) & Nielsen, K. (Peer reviewer)
7. Jan 2013

ChemPhysChem (Journal)
Kongsted, J. (Peer reviewer)
2014

ChemPhysChem (Journal)
Kongsted, J. (Peer reviewer)
2014

Cogent Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2015

Cogent Chemistry (Journal)
Kongsted, J. (Peer reviewer)

2016

International Journal of Quantum Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2009

International Journal of Quantum Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2010

International Journal of Quantum Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2010

Introduction to Car-Parinello methods using CPMD
Kongsted, J. (Organizer)
21. Jan 2010 → 22. Jan 2010

Journal of Chemical theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2013

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Editor)
1. Jan 2009

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2011

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2011

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2012

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2012

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2013

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2013

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2014

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2014

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2014

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2014

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2015

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2016

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2016

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2016

Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2017

Journal of Molecular Structure: THEOCHEM (Journal)
Kongsted, J. (Editor)
1. Jan 2009

Journal of Molecular Structure: THEOCHEM (Journal)
Kongsted, J. (Editor)
1. Jan 2009

Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2017

Journal of Physical Chemsitry (Journal)
Kongsted, J. (Peer reviewer)
2015

Journal of Physical Chemsitry (Journal)
Kongsted, J. (Peer reviewer)
2016

Journal of Physics: Condensed Matter (Journal)
Kongsted, J. (Editor)
1. Jan 2009

Københavns Universitet
Kongsted, J. (Supervisor)
28. Oct 2010

Ligh-Harvesting and Quantum Chemistry
Kongsted, J. (Lecturer)
19. Mar 2009

Linköping University (External organisation)
Kongsted, J. (Member)
Mar 2012

Magnetic Resonance in Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2012

Magnetic Resonance in Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2012

Molecular Physics (Journal)
Kongsted, J. (Peer reviewer)
2013

Molecules (Journal)
Kongsted, J. (Peer reviewer)
2014

Molecules (Journal)
Kongsted, J. (Peer reviewer)
2014

Multiscale Modelling and Simulation in Science : Project leader for computational exercise
Kongsted, J. (Organizer)
5. Nov 2009 → 12. Nov 2009

PCCP (Journal)
Kongsted, J. (Peer reviewer)
2011

PCCP (Journal)
Kongsted, J. (Peer reviewer)
2011

PCCP (Journal)
Kongsted, J. (Peer reviewer)
2012

PCCP (Journal)
Kongsted, J. (Peer reviewer)
2015

PCCP (Journal)
Kongsted, J. (Peer reviewer)
2015

PCCP (Journal)
Kongsted, J. (Peer reviewer)
2016

Ph.D. Bedømmelsesudvalg (External organisation)
Kongsted, J. (Member)
15. Aug 2009 → 1. Oct 2009

Physical Chemistry Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2018

Physical Chemistry Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2018

Physical Chemistry Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2018

Physical Chemistry Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2018

Physical Chemistry Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2018

Physical Chemistry Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2018

Quantum Chemical Studies of Photoactive Proteins
Kongsted, J. (Lecturer)
25. Jun 2010

Research Interests
Kongsted, J. (Lecturer)
20. Feb 2009

The 15th European Seminar on Computational Methods in Quantum Chemistry
Kongsted, J. (Participant)
16. Jun 2011 → 19. Jun 2011

The Journal of Chemical Physics (Journal)
Kongsted, J. (Editor)
1. Jan 2010

The Journal of Chemical Physics (Journal)
Kongsted, J. (Editor)
1. Jan 2010

The Journal of Chemical Physics (Journal)
Kongsted, J. (Editor)
1. Jan 2010

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2012

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
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The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
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The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
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The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
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The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
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The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
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The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2015

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2015

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2017

The Journal of Chemical Physics (Journal)
Kongsted, J. (Peer reviewer)
2018

The Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Editor)
1. Jan 2010

The Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2012

The Journal of Chemical Theory and Computation (Journal)
Kongsted, J. (Peer reviewer)
2018

The Journal of Physical Chemistry B (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Physical Chemistry B (Journal)
Kongsted, J. (Peer reviewer)
2014

The Journal of Physical Chemistry B (Journal)
Kongsted, J. (Peer reviewer)
2014

The Journal of Physical Chemistry B (Journal)
Kongsted, J. (Peer reviewer)
2018

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2009

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2009

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2009

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2010

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2010

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Editor)
1. Jan 2010

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2011

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2012

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2013

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2013

The Journal of Physical Chemistry (Journal)
Kongsted, J. (Peer reviewer)
2017

The Journal of Physical Chemistry Letters (Journal)
Kongsted, J. (Editor)
1. Jan 2010

The Journal of Physical Chemistry Letters (Journal)
Kongsted, J. (Peer reviewer)
2016

The Journal of Physical Chemistry Letters (Journal)
Kongsted, J. (Peer reviewer)
2018

The Journal of Physical Chemistry Letters (Journal)
Kongsted, J. (Peer reviewer)
2018

Theoretical Chemistry Accounts (Journal)
Kongsted, J. (Peer reviewer)
2017

UiT The Arctic University of Norway
Kongsted, J. (Visiting researcher)
26. Jun 2010 → 1. Jul 2010

UiT The Arctic University of Norway (External organisation)
Kongsted, J. (Member)
1. Jun 2009 → 31. Aug 2009

Universitetspædagogikum
Kongsted, J. (Participant)
11. Jan 2010 → 13. Jan 2010

Universitetspædagogikum
Kongsted, J. (Participant)
18. Aug 2010 → 19. Aug 2010

University of Copenhagen: Master thesis opponent
Kongsted, J. (Examiner)
4. Dec 2009

University of Pisa
Kongsted, J. (Visiting researcher)
24. Apr 2009 → 2. May 2009

University of Pisa
Kongsted, J. (Visiting researcher)
9. Dec 2009 → 12. Dec 2009

University of Pisa
Kongsted, J. (Visiting researcher)
31. Jul 2010 → 7. Aug 2010

University of Pisa
Kongsted, J. (Visiting researcher)
25. Jul 2011 → 5. Aug 2011

Vibrational Spectroscopy (Journal)
Kongsted, J. (Editor)
1. Jan 2010

Vibrational Spectroscopy (Journal)
Kongsted, J. (Peer reviewer)
22. Sept 2010 → …

WATOC
Kongsted, J. (Participant)
16. Jul 2011 → 22. Jul 2011

Teaching Portfolio

**Educational Training
Master of Science, August 2001, University of Copenhagen, Denmark.
PhD February 2005, University of Copenhagen, Denmark
Universitetspædagogikum (Lecturer Training Programme), December 2010, University of Southern Denmark (SDU)
One-day course on E-learning, SDU, March 2010
One-day course on project based learning, SDU, March 2010
One-day course on ”the good lecture”, SDU, Mai 2010
One-day course on teaching methods within natural sciences, SDU, October 2010
Two-day course on PhD supervision, SDU, January 2012
FESTA: Study circle on PhD supervision and gender, 2014 – 2015 (4 meetings)
**Educational administrative experience
Since January 2013 member of the teaching board at the Department of Physics, Chemistry and Pharmacy, SDU.
Member of the eScience Center Board and herein engaged in the eScience Center teaching activities / courses.
Supervisor in relation to the SDU Lecturer Training Programme.
Course responsibility in courses on computational chemistry, molecular modeling and mathematical methods for chemists.
Head of the PhD school at Nat SDU (2015 -)
**Overall teaching philosophy
My overall teaching philosophy is very simple: “You don’t learn how to ride a bike by looking at your neighbor doing it”. Only by actively participate, commit and explore you will succeed in learning. Thus, my overall teaching philosophy aims at bringing as much as possible the students in action. In practical terms this means that my teaching is generally built around a short introduction of the new material (in more advanced courses some of the highly motivated students are encouraged to do this with proper feedback from me), and hereafter I let the students work with this material in form of well-structured practical, computational or theoretical exercises with feedback from both me as well as the students themselves. In this phase of the teaching I see my main function as consulter. I never provide the students with “the solution” but rather guide them in finding this themselves.
**Teaching experience
Laboratory (computer) and theoretical exercises, lectures, course responsibility and conduction of exams in
1)Computational and theoretical chemistry
2)Reaction dynamics, laser chemistry and optics
3)Molecular modeling
4)Quantum chemistry
5)Mathematical methods for chemistry students
6)General chemistry
Courses in which I have been either responsible or contributing teacher at SDU includes:
KE534/803 – Molecular modeling (5 ECTS) – lectures, exercises and computer exercises.
KE533/820/821 – Advanced computational quantum chemistry and theoretical spectroscopy (5/10 ECTS) - lectures, exercises and computer exercises.
KE529 – Mathematical methods for chemistry and nanobioscience (5 ECTS) - lectures, exercises and computer exercises.
KE522 – Quantum chemistry and spectroscopy (10 ECTS) - lectures, exercises and computer exercises.
KE531 – Project in computational chemistry (5 ECTS) – lectures, exercises, computer exercises and supervision.
FF503 – General chemistry (20 ECTS in total) – exercises and computer exercises
FF501 – First year science project (10 ECTS) – lectures, computer exercises and supervision.
BMB834 – Advanced course in modeling and protein structures (5 ECTS) – lectures, exercises, computer exercises and supervision.
I have experience with both oral, written and project exams.
**Supervision
7 project students in computational chemistry University of Copenhagen (2003-2006)
Project student Sanne Sander Rasmussen (supervisor 2010)
Project student Nanna holmgaard List (supervisor 2010)
Project student Kaspar Rasmussen (supervisor 2011)
Project student Signe Irminger (supervisor 2014)
Project student Marie-Louise Jæger Hovgaard Pedersen (co-supervisor 2014)
Project student Thomas Pabst Gunnarsson (supervisor 2015)
Project student Mogens Buse (supervisor 2016)
Project student Nina Junager (co-supervisor 2016)
Project student Frederik Juel Larsen (supervisor 2016)
Project student Lutje Joensen (supervisor 2017)
Project student Frederik Kamper Jørgensen (supervisor 2018)
Bachelor student Nanna Holmgaard List (supervisor 2010)

Bachelor student Lina Johanna Nåbo (co-supervisor 2012)
Bachelor student Christina Wegeberg (co-supervisor 2012)
Bachelor student Jehan Annan Sulayman Goreal (supervisor 2013)
Bachelor student Abdirazak Ali Sheikh Hussein (supervisor 2013)
Bachelor student Admir Osmanovic (supervisor 2013-2014)
Bachelor student Ibrahim Dahir Hanaf (supervisor 2015)
Bachelor student Maria Karlsen (supervisor 2015)
Bachelor student Abdishakur Mohamed Abdirahman (supervisor 2016)
Bachelor student Erik Kjellgren (supervisor 2016)
Bachelor student Oliver Glue (supervisor 2016)
Bachelor student Peter Reinholdt (supervisor 2016)
Bachelor student Martin Elberg (supervisor 2018)
Bachelor student Julie Egholm (supervisor 2018)
Bachelor student Julie Hansen (supervisor 2018)
Bachelor student Lutje Joensen (supervisor 2018)
Bachelor student Signe Wind (supervisor 2018)
Bachelor student Laust Moesgaard (supervisor 2019)
Bachelor student Frederik Kamper Jørgensen (supervisor 2019)
Bachelor student Cecilie Kofod (supervisor 2019)
Master Student Kestutis Aidas (co-supervisor 2005-2006)
Master student Andreas Møgelhøj (co-supervisor 2006-2007)
Master student Jógvan Magnus Olsen (co-supervisor 2008-2009)
Master student Anne Sørensen (co-supervisor 2009-2010)
Master student Kaspar Rasmussen (supervisor 2011 – 2012)
Master student Nicolai Mathias Trædholm (supervisor 2013-2014)
Master student Marie-Louise Jæger Hovgaard Pedersen (co-supervisor 2014-2015)
Master student Thomas Pabst Gunnarsson (supervisor 2015-2017)
Master student Mogens Peter Andersen Buse (co-supervisor 2016-2017)
Master student Trine Djurhuus (supervisor 2018)
Master student Lutje Joensen (supervisor 2018-19)
Ph.D. student Kestutis Aidas (co-supervisor 2007-2010)
Ph.D. student Arnfinn Hykkerud Steindal UiT (guest Ph.D. student at SDU 2009)
Ph.D. student Karina Ebbesen Jessen KU (guest Ph.D. student at SDU 2009-2011)
Ph.D. student Hannah Kjær KU (guest Ph.D. student at SDU 2009-2012)
Ph.D. student Jógvan Magnus Olsen (supervisor 2009-2012)
Ph.D. student Erik Donovan Hedegård (supervisor 2010-2013)
Ph.D. student Nanna Holmgaard List (supervisor 2011-2015)
Ph.D. student Sarah Witzke (supervisor 2012-2015)
Ph.D. student Morten Nørby Pedersen (supervisor 2012-2015)
Ph.D. student Lina Johanna Nåbo (supervisor 2013-2017)
Ph.D. student Selvaraj Sengotiyan (supervisor 2014-2017)
Ph.D. student Julie Stendevad (supervisor 2015-2018)
Ph.D. student Peter Reinholdt (supervisor 2017-2021)
Ph.D. student Salvatore Prioli (supervisor 2017-2021)
Post Doc Jógvan Magnus Olsen (supervisor 2012-2013)
Post Doc Casper Steinamnn Svendsen (supervisor 2012-2013)
Post Doc Vasanthanathan Poongavanam (supervisor 2013-2015)
Post Doc Erik Donovan Hedegård (supervisor 2014)
Post Doc Nanna Holmgaard List (supervisor 2015-2016)
Post Doc Morten Sten Nørby (supervisor 2015-2018)
Post Doc Dalibor Hrsak (supervisor 2016-2018)
**Master and Bachelor thesis opponent
I frequently act as opponent in relation to either Bachelor or Master thesis defends at other Danish universities.
**PhD opponent
University of Tromsø, Norway, November 2007
University of Linkobing, Sweden, March 2012
University of Copenhagen, February 2013
University of Southern Denmark (chairman), February 2015
University of Alberta, Canada, August 2016
University of Pisa, Italy, November 2016
University of Copenhagen, January 2018
University of Southern Denmark (chairman), November 2018
**Student evaluations in regards to teaching
During my time at the University of Southern Denmark I have always received positive feedback from student evaluations. In my evaluations I have been described as being a good communicator, having a high professional level, very committed to student learning, as well as having good teaching abilities and a good planning of the teaching.

**Reflections on my teaching including my use of methods, materials and tools

My use of teaching methods, materials and tools depend very much on the specific type of teaching. My experience is that it is mandatory always to begin by setting the frames for a given course: What do I expect from the students and what can the students expect from me? I believe this is a simple but often forgotten point. The form used in my teaching varies between short lectures (in my experience 45 minutes for a lecture is too long, and I usually aim for lectures of only 15-20 minutes) where new material is introduced followed by problem based learning in the form of either theoretical, computational or experimental exercises. In this phase of the teaching the students work with the details I have left out in my intro and overview lectures, e.g. specific derivations and connections between expressions introduced by me. In addition, I include in many courses a project phase where the students work either individually or in smaller groups on a project they have defined themselves. Naturally, in this phase of the teaching feedback from the teacher is a very important component of the student learning. My experience is that the problem formulation phase is very time consuming, but also highly motivating and instructive for the students. We often train the students in solving a given problem, but I try (also) to train the students in problem formulations, i.e. to take something unconcrete and make this concrete and formulate how this concrete problem can be solved by the methods the students have learned in a given course. By this, I believe that it is important not only to train the students in solving standard exercises, but also to encourage them to think in new terms and ways – and to take risks. Also my experience with project based exams is very good and highly recommended, especially for the more advanced courses.

In the academic year 2014-2015 I took a new initiative in form of introducing video lectures in my teaching. My motivation for this was two-fold: First of all, I wanted to see if video lectures would affect in positive terms the students preparation before coming to class. Second, I wanted to shift to a form for teaching where I created more possibilities for student activation and participation in class, as well as creating more time for me to interact directly with the students. The video lectures were used in the way that I – before class – prepare and upload a video to YouTube going through the intro material for the given lecture. The duration of these video lectures are between 10 and 15 minutes. The students are expected to watch these videos before coming to class and to prepare a number of questions to the material. In the video only the most important material is presented leaving out many of the details and derivations. Instead these are formulated as “exercises” and in the class the students work through these exercises (with my help and guiding). My experience with this form of “flipped classroom” teaching is indeed very positive and definitely something I will further develop in the future. First of all, this form for teaching provides a lot of time for the teacher to actually work with the students, and as a teacher you get the joy of experiencing that the students meet to class prepared. As an example of this, I experienced that by changing to this teaching form I could cover more teaching material than I would otherwise have been able to do. Furthermore, due to the fact that the students worked in detail with the material, the quality of the teaching and learning improved markedly: I have never before had a class with such many (intelligent) questions, general interest for the subject and clearly this class achieved a very high level of understanding of the material. I evaluated this form for teaching given to a class on the subject of “Molecular Modeling” (and a few times to a class on the subject of “Mathematics in Chemistry”) through small and informal focus interviews as well as a written evaluation and the response was very positive. The students liked very much this form for teaching and encouraged this to be implemented in more courses. Most importantly – I could see that it worked and lead to a higher understanding of the material.

In summary, I can clearly recommend this form for teaching. A warning: creating the videos takes a lot of time and in order for the students to take these serious they should possess a high quality.

**Student supervision

Over time, I have acted as supervisor for a fairly large number of students both at the undergraduate and graduate level. In addition, I have supervised a number of post docs. I always devote a large amount of time to supervision tasks since I find this to be a very important aspect of my job: to educate the next generation of researchers. I always prepare for scheduled supervision meetings and do my best in order to meet the students “where they are” in their scientific development. As an indication (and indeed only an indication) of my supervisor abilities, I here mention that PhD students and post docs under my supervision generally have performed very well and received several prices/awards including Villum Fonden, Carlsberg and Research Council post doc fellowships, Sapere Aude awards as well as a Zonta award. Devoting time to help students in planning their carrier is indeed a very important aspect of my job and something I highly prioritize.

**Development of courses and teaching materials

Since I was first employed at SDU, I have been the driving force in respect to strengthening of the theoretical/computational part of the chemistry education at the Department of Physics, Chemistry and Pharmacy. This is a process that is still ongoing and an area in which I definitely will be active in the future. For this, I have been – and still am – developing courses in molecular modeling, mathematical methods for chemists, quantum chemistry, symmetry and spectroscopy as well as restructuring existing courses on quantum chemistry. In particular, I have in these courses developed a significant amount of teaching material especially related to theoretical and computer exercises which, in my experience, have lead to a better understanding of these subjects that are generally found difficult by the students. For me, it is very clear that the use of theoretical and computer exercises both motivates and brings up central student questions related to the learning process that would otherwise not have been brought up. Also, for a student, there is nothing as motivating as the feeling of success upon being able to understand and solve a challenging exercise.

Recently, I took up the challenge of developing a new (Bachelor) course on mathematical methods for chemists. Among the chemistry teachers it was a general concern that the mathematical skills of our chemistry students was at a too low level with a negative consequence of the students learning. Thus, in order to raise the general mathematical level among our students, I designed a new mandatory course on mathematical methods for chemists. In addition to traditional lectures (and video lectures) and exercises this course consists of a large amount of computer exercises where the students learn how to use mathematical software in order to solve rather complex chemical problems (e.g. solving coupled differential equations to describe chemical kinetics), thereby bringing the mathematical methods in play in a clear context for the

chemistry students. Due to the high degree of student activation as well as a clear connection between the taught mathematical methods and chemistry, this course was very successful as clearly seen from the positive student evaluation. Furthermore, I have very recently designed an elective module on computational chemistry as part of the chemistry Bachelor education. This module will clearly strengthen the education within computational chemistry at SDU as well as the chemistry education in general. Furthermore, such a module will better – and in a much more clear way - make it possible for students to achieve a Master's degree in interdisciplinary sciences, e.g. to link to the activities/education related to the eScience Center, as well as other disciplines.