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RESEARCH INTERESTS

Simulation of complex chemical systems, nonadiabatic processes, light-matter interactions, strong-field induced electron dynamics, linear and nonlinear spectroscopies, nondipolar effects.

EDUCATION

PhD, Theoretical Chemistry, University of Southern Denmark, Denmark. **2011 – 2016**
Thesis title: Theoretical Description of Electronic Transitions in Large Molecular Systems in the Optical and X-Ray Regions (degree received: 01/26/2016).
Supervisors: Prof. Jacob Kongsted and Prof. Hans Jørgen Aa. Jensen.

M.Sc. of Honors, Interdisciplinary Science Studies, University of Southern Denmark, Denmark. **2010 – 2013**
Thesis title: Facing the Challenges of Polarizable-Embedded Molecules in Molecular Biophotonics (defense date: 07/09/2013).
Supervisor: Prof. Jacob Kongsted.
(GPA 12.0/12.0).

B.Sc., Chemistry, University of Southern Denmark, Denmark. **2007 – 2010**
(GPA 12.0/12.0).

ACADEMIC EXPERIENCE

VILLUM postdoctoral fellow with Prof. Todd Martínez, **Sept. 2017–present**
Stanford University, USA.
Topic: Computational photodynamics and advanced X-Ray spectroscopies of complex molecular systems.

Individual Carlsberg fellow visiting Prof. Patrick Norman, **Feb. 2016 – Aug. 2017**
KTH Royal Institute of Technology, Sweden.
Topic: Targeting conformational changes in DNA with X-ray natural circular dichroism.

Research assistant with Prof. Jacob Kongsted, **Aug. 2015 – Jan. 2016**
University of Southern Denmark, Denmark.
Topic: Open-ended response theory with polarizable embedding.

AWARDS AND GRANTS

1st Poster Prize Award **2018**
Title: *Nonadiabatic Electron Dynamics with Full Multiple Spawning*
West Coast Theoretical Chemistry Symposium (Stanford, USA).

VILLUM Foundation Postdoctoral fellowship (1,154,000 DKK≈176,000 USD) **2017**
The VILLUM Foundation.

Individual Carlsberg fellowship (350,000 DKK≈53,000 USD) **2016**
The Carlsberg Foundation.

The Danish Natural Science Academy PhD Award **2016**
for an extraordinary excellent Danish PhD thesis within natural sciences.
The Danish Natural Science Academy.

Individual Carlsberg fellowship (350,000 DKK≈53,000 USD) **2015**
The Carlsberg Foundation.

EliteForsk PhD Travel Grant (300,000 DKK≈45,800 USD) **2014**
The Danish Council for Independent Research.

Zonta Denmark PhD Award (50,000 DKK≈7,600 USD) **2013**
for an outstanding woman in natural sciences and technology.
Zonta Denmark.

Travel Grant (12,000 DKK≈1,800 USD) **2011**
The Danish Chemical Society.

SOFTWARE CONTRIBUTIONS

Software co-authorships

The quantum chemistry program DALTON (http://www.daltonprogram.org/): Main contributions are concerned with the development of the full semi-classical light–matter interaction operator as well as polarizable environment models in a coupled-cluster linear response framework.

The polarizable embedding (PE) library (https://gitlab.com/pe-software/pelib-public/): Main contributions concern the development of routines for describing the coupling between a chromophore, its environment and an external perturbation (electric or geometric) within a response formulation.

ORGANIZATION OF MEETINGS

Co-organizer (with Hans Aagren) of the symposium "A Voyage from Nonlinear Optics to Biophotonics – joining Theory and Experiment", Stockholm, Sweden. https://sites.google.com/view/noab2018/ **2018**

ORAL PRESENTATIONS

Ab Initio Probing of Photodynamics with Transient X-Ray Absorption (invited) **May 10, 2019**
D. E. Shaw Graduate and Postdoc Research Forum, New York, USA.

Parallel Multiple Spawning (contributed) **March 30, 2018**
TeraChem/FMS Developer's Meeting, Stanford, USA.

Probing DAPI-DNA Interactions by means of Circularly Polarized Light (contributed) **April 11, 2017**
Molecular Properties and Computational Spectroscopy.
Conference, CNR Research Area, Pisa, Italy.

Addressing Local Electric Fields with Polarizable Embedding (invited) **Nov. 2, 2016**
Department of Chemistry, East China University of Science and Technology.
Theoretical chemistry workshop, Shanghai, China.

Electronic Transitions in Large Molecular Systems with Polarizable Embedding (seminar) **July 22, 2016**
Department of Chemistry, Penn State University, USA.

Optical Properties and Excited States of Large Molecular Complexes using a Polarizable-Embedding Approach (seminar) **Aug. 14, 2014**
Beckmann Institute, University of Illinois at Urbana-Champaign, USA.

Optical Properties and Excited States of Large Molecular Complexes using a Polarizable-Embedding Approach (seminar) **July 21, 2014**
Department of Chemistry, University of Calgary, Canada.

One- and Two-Photon Absorption Properties of the miniSOG Protein (invited) **Nov. 2, 2012**
Meeting at Centre for Oxygen Microscopy and Imaging (COMI), Aarhus University, Denmark.

POSTER PRESENTATIONS

Ab Initio Probing of Photodynamics with Transient X-Ray Absorption **May 19, 2019**
Northern California Theoretical Chemistry Meeting, Berkeley, USA.

Ab Initio Probing of Photodynamics with Transient X-Ray Absorption **May 10, 2019**
D. E. Shaw Graduate and Postdoc Research Forum, New York, USA.

Nonadiabatic Electron Dynamics with Full Multiple Spawning **March 28, 2018**
West Coast Theoretical Chemistry Symposium, Stanford, USA.

Electronic Transitions in Complex Molecular Systems: Addressing Local Electric Fields with Polarizable Embedding **Nov. 7, 2016**
Excited States Simulations: Bridging Scales, Marseille, France.

Linear Absorption beyond the Electric-Dipole Approximation **June 28, 2016**
8th Molecular Quantum Mechanics, Uppsala, Sweden.

TEACHING EXPERIENCE

Teaching activities, including design and preparation of course material, University of Southern Denmark, Denmark.

- Advanced Quantum Chemistry **2014**
- Introductory Quantum Chemistry **2014 – 2015**
- Mathematical Methods in Chemistry **2013**
- Electromagnetism **2012**

– Introductory Chemistry **2010 – 2013**
– Biochemistry **2009 – 2010**

Mentoring of students **2013 – 2015**
Mentoring of three PhD students.
(resulted in publications [6], [7], [9], [17] and [18]).

Solution Manual to *Molecular Electromagnetism — A Computational Chemistry Approach*, *Oxford University Press,* **2015**
S. P. A. Sauer, R. Faber, N. H. List, K. Mackeprang, N. Wahlberg and M. Simmermacher.

OUTREACH

Quantum-Mechanical Microscope Reveals Molecular Mechanisms. **2014**
N.H. List, J. Kongsted, *Dansk Kemi*, 95, 24, 2014.
http://www.kemifokus.dk/kvantekemisk-mikroskop-afsloerer-molekylaere-mekanismer/ (accessed 01/05/19).

Rational Design of Biomarkers based on Theoretical Chemistry **Nov. 13, 2013**
Popular scientific talk for general audience.
University of Southern Denmark, Denmark.

Unraveling Reaction Mechanisms by means of Computational Chemistry **2010 – 2014**
Co-organized, designed and executed computational chemistry two-hours exercises as part of event days for students in upper secondary school/high school, University of Southern Denmark, Denmark.

PUBLICATIONS

[1] L. Konecky, N. H. List, P. Norman, M. Repísky
Assessment of the Importance of Relativistic Effects in X-Ray Circular Dichroism: An RT-TDDFT Study.
In preparation.

[2] N. H. List, T. Melin, T. Saue.
Beyond the Electric-Dipole Approximation in Relativistic Simulations of X-ray Absorption Spectroscopy.
In preparation [corresponding author].

[3] N. H. List, M. Ringholm, P. Norman.
Response Theory for Pulses.
In preparation [corresponding author].

[4] N. H. List, J. Knoops, J. Rubio-Magnieto, J. Idé, D. Beljonne, P. Norman, M. Surin, M. Linares.
Origin of DNA-Induced Circular Dichroism in a Minor-Groove Binder.
J. Am. Chem. Soc. **2017**, 139, 14947.

[5] N. H. List, P. Norman, J. Kongsted, H. J. Aa. Jensen.
A Quantum-Mechanical Perspective on Linear Response Theory within Polarizable Embedding.
J. Chem. Phys. **2017**, 146, 234101 [corresponding author].

[6] N. H. List, T. Saue, P. Norman.
Rotationally Averaged Linear Absorption Spectra Beyond the Electric-Dipole Approximation.
Mol. Phys. **2017**, 115, 63 [corresponding author].

[7] L. J. Nåbo, N. H. List, C. Steinmann, J. Kongsted.
A Computational Approach to Evaluation of Optical Properties of Membrane Probes.
J. Chem. Theory Comput. **2017**, 13, 719.

[8] S. Witzke, N. H. List, J. M. H. Olsen, C. Steinmann, M. Petersen, M. T. P. Beerepoot, J. Kongsted.
An Averaged Polarizable Potential for Multiscale Modeling in Phospholipid Membranes.
J. Comput. Chem. **2017**, 5, 601.

[9] H. Steindal, M. T. P. Beerepoot, M. Ringholm, N. H. List, K. Ruud, J. Kongsted, J. M. H. Olsen. Open-ended Response Theory with Polarizable Embedding: Multiphoton Absorption in Biomolecular systems.
Phys. Chem. Chem. Phys. **2016**, 18, 28339.

[10] L. J. Nåbo, J. M. H. Olsen, N. H. List, L. M. Solanko, D. Wüstner, J. Kongsted.
Embedding beyond Electrostatics – The Role of Wave-Function Confinement.
J. Chem. Phys. **2016**, 145, 104102.

[11] N. H. List, J. M. H. Olsen, J. Kongsted.
Excited states in Large Molecular Complexes Through Polarizable Embedding.
Phys. Chem. Chem. Phys. **2016**, 18, 20234.

[12] Reese,* N. H. List,* J. Kongsted, I. Solov'yov.
How far does a Receptor Influence the Vibrational Properties of an Odorant?
PloS One **2016**, DOI: 10.1371/journal.pone.0152345.

[13] M. T. P. Beerepoot, A. H. Steindal, N. H. List, J. Kongsted, J. M. H. Olsen.
Averaged Solvent Embedding Potential Parameters for Multiscale Modeling of Molecular Properties.
J. Chem. Theory Comput. **2016**, 12, 1684.

[14] N. H. List, H. J. Aa. Jensen, J. Kongsted.
Local Electric Fields and Molecular Properties in Heterogeneous Environments Through Polarizable Embedding.
Phys. Chem. Chem. Phys. **2016**, 18, 10070 [corresponding author].

[15] M. T. P. Beerepoot, D. Friese, N. H. List, J. Kongsted, K. Ruud.
Benchmarking Two-Photon Absorption Cross Sections: Performance of CC2 and CAM-B3LYP.
Phys. Chem. Chem. Phys. **2015**, 17, 19306

[16] N. H. List, R. Zaleśny, N. A. Murugan, J. Kongsted, W. Bartkowiak, H. Ågren.
Relation between Nonlinear Optical Properties of Push–Pull Molecules and Metric of Charge Transfer Excitations.
J. Chem. Theory Comput. **2015**, 11, 4182.

[17] N. H. List, J. Kauczor, T. Saue, H. J. Aa. Jensen, P. Norman.
Beyond the Electric-Dipole Approximation: A Formulation and Implementation of Molecular Response Theory for the Description of Absorption of Electromagnetic Field Radiation.
J. Chem. Phys. **2015**, 142, 244111 [corresponding author].

[18] L. J. Nåbo, N. H. List, S. Witzke, D. Wüstner, H. Khandelia, J. Kongsted.
Design of New Fluorescent Cholesterol and Ergosterol Analogs: Insights from Theory.
Biochim. Biophys. Acta **2015**, 1848, 2188.

[19] D. Hršak, L. Holmegaard, A. S. Poulsen, N. H. List, J. Kongsted, M. P. Denofrio, R. Erra-Balsells, F. M. Cabrerizo, O. Christiansen, P. R. Ogilby.
Experimental and Computational Study of Solvent Effects on One- and Two-Photon Absorption Spectra of Chlorinated Harmines.
Phys. Chem. Chem. Phys. **2015**, 17, 12090.

[20] J. M. H. Olsen, N. H. List, K. Kristiansen, J. Kongsted.
Protein Embedding Potentials: An Analysis in Terms of Electrostatic Potentials.
J. Chem. Theory Comput. **2015**, 11, 1832.

[21] N. H. List, M. T. P. Beerepoot, J. M. H. Olsen, B. Gao, K. Ruud, H. J. Aa. Jensen, J. Kongsted.
Molecular Quantum Mechanical Gradients within the Polarizable Embedding Approach — Application to the Internal Vibrational Stark Shift of Acetophenone.
J. Chem. Phys. **2015**, 142, 034119 [corresponding author].

[22] N. H. List, S. Coriani, J. Kongsted, O. Christiansen. Lanczos-Driven Coupled Cluster Damped Linear Response Theory for Molecules in Polarizable Environments.
J. Chem. Phys. **2014**, 141, 244107 [corresponding author].

[23] M. Pourmousa, R. Tomasz, R. Mikkeli, I. Vattulainen, L. M. Solanko, D. Wüstner, N. H. List, J. Kongsted, M. Karttunen.
Dehydroergosterol as an Analogue for Cholesterol: Why it Mimics Cholesterol so well or does it.
J. Phys. Chem. B **2014**, 118, 7345.

[24] N. H. List, S. Coriani, O. Christiansen, J. Kongsted.
Identifying the Hamiltonian Structure in Linear Response Equations.
J. Chem. Phys. **2014**, 140, 224103 [corresponding author].

[25] N. H. List,* F. M. Pimenta,* L. Holmegaard, R. J. Jensen, M. Etzerodt, J. Kongsted, O. Christiansen, P. R. Ogilby.
Effect of Chromophore Encapsulation on Linear and Non-Linear Optical Properties: The Case of 'miniSOG', a Protein-Encased Flavin.
Phys. Chem. Chem. Phys. **2014**, 16, 9950.

[26] N. H. List, C. Curutchet, S. Knecht, B. Mennucci, J. Kongsted.
Toward Reliable Prediction of the Energy Ladder in Multichromophoric Systems: A Benchmark Study on the FMO Light-Harvesting Complex.
J. Chem. Theory Comput. **2013**, 9, 4928 [corresponding author].

[27] E. D. Hedegård, N. H. List, H. J. Aa. Jensen, J. Kongsted.
The Multi-Configuration Self-Consistent Field Method within a Polarizable Embedded Framework.
J. Chem. Phys. **2013**, 139, 044101.

[28] N. H. List, H. J. Aa. Jensen, J. Kongsted, E. D. Hedegård.
A Unified Framework for the Polarizable Embedding and Continuum Methods within Multiconfigurational Self-Consistent Field Theory.
Adv. Chem. **2013**, 66, 195.

[29] N. H. List, J. M. H. Olsen, A. H. Steindal, H. J. Aa. Jensen, J. Kongsted.
Molecular-Level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore.
J. Phys. Chem. Lett. **2012**, 3, 3513.

[30] Dreier, S. Kumar, H. Søndergaard, M. L. Rasmussen, L. H. Hansen, N. H. List, J. Kongsted, B. Vester, P. Nielsen.
A Click Chemistry Approach to Pleuromutilin Derivatives, Part 2: Conjugates with Acyclic Nucleosides and their Ribosomal Binding and Antibacterial Activity.
J. Med. Chem. **2012**, 55, 2067.

[31] N. H. List, J. M. H. Olsen, T. Rocha-Rinza, O. Christiansen, J. Kongsted.
Performance of popular XC-Functionals for the Description of Excitation Energies in GFP-Like Chromophore Models.
Int. J. Quantum Chem. **2012**, 112, 789.
*Co-first author