Henrik R. Larsson

Curriculum Vitae

California Institute of Technology
Division of Chemistry and Chemical Engineering
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Theoretical Chemist

Professional Experiences

since Sept 2018 **Postdoctoral Scholar**, *California Institute of Technology, USA*.

May 2018–Sept 2018 **Postdoctoral Scholar**, *Kiel University, Germany*.

Dec. 2014–May 2018 **Research Associate**, *Kiel University, Germany* and *Weizmann Institute of Science, Rehovot, Israel*.

2013 **Research Assistant**, *Jülich Supercomputing Center*, Guest Student Program.

Education

Dec. 2014–May 2018 **PhD in Theoretical Chemistry**, *Kiel University, Germany* and *Weizmann Institute of Science, Rehovot, Israel*, with distinction (summa cum laude).

2013–2014 **Master of Science (Chemistry)**, *Kiel University, Germany*, final grade 1.0 (1.0 is best, 4.0 is worst), best student of the year.

2013 **Guest Student Program**, *Jülich Supercomputing Center*, three-month scientific project.

2012–2013 **Visiting Master's Student**, *Lund University, Sweden*.

2009–2012 **Bachelor of Science (Chemistry)**, *Kiel University, Germany*, final grade 1.1, best student of the year.

2009 **Secondary School**, *Domschule Schleswig*, final grade 1.1, best pupil of the year.

Research

Postdoctoral Studies

Title *Applying tensor decompositions to strongly correlated quantum systems*

Supervisor Prof. Garnet K.-L. Chan (Theoretical Chemistry, California Institute of Technology)

Description Method development and applications in electronic structure and vibrational spectra calculations. Development of methods based on tensor-network states (TNSs) in order to efficiently simulate strongly correlated quantum systems. Connections between TNSs and simple methods such as valence bond are explored.

PhD Thesis

Title *Efficient approaches to multidimensional quantum dynamics*

Supervisors Prof. Bernd Hartke (Theoretical Chemistry, Kiel University) and
Prof. David J. Tannor (Chemical Physics, Weizmann Institute of Science)

Stays in Israel: Dec. 2014 to May 2015 and Oct. 2016 to May 2017.

Description Method development and applications in theoretical quantum dynamics. The time-dependent Schrödinger equation is solved by using efficient dynamical pruning of the wavefunction with localized basis functions. Compared to conventional methods, speed-ups of up to 50 are achieved for up to 24-dimensional systems. Applications are in the fields of chemical reaction dynamics, nonadiabatic vibrational dynamics and the control of electron dynamics in strong laser fields.

Master's Thesis

Title *Laser-induced correlated electron dynamics in small molecules*

Supervisors Prof. Michael Bonitz and Dr. Sebastian Bauch (both Theoretical Physics, Kiel Univ.)

Description Method development and applications in strong-field electron dynamics. Implementation of a sophisticated finite-element/grid-based basis and coordinates well-suited for studying diatomics in a time-dependent multi-reference configuration-interaction code. Exploration of correlation effects in the photoelectron angular distributions for tunneling and above-threshold ionization of the molecule LiH for short and intense laser fields.

Guest Student Program

Title *Molecular orbital generation sequences*

Supervisor Dr. Thomas Müller, main developer of the Columbus quantum chemistry program (Jülich Supercomputing Center)

Description Method development in electronic structure theory. Development of software tools for computing orbital projections between basis sets, similar structures, point groups, orbital rotations in real space, and the assembling of molecular orbitals from fragments. This works for arbitrary quantum chemistry packages and requires a minimal set of information.

Bachelor's Thesis

Title *Global Optimization of Parameters for the Reactive Force Field ReaxFF*

Supervisor Prof. Bernd Hartke (Theoretical Chemistry, Kiel Univ.)

Description Method development in molecular modeling. Global parametrization of the reactive force field ReaxFF for silicon-based systems, and the development of a new force field for azobenzene, using evolutionary algorithms. Exploration of the best strategies on how to perform global optimization of high-dimensional (>60 dimensions) and complex fitness landscapes.

Teaching Experience

2019 Attending a 10-week course on "Principles of University Teaching and Learning in STEM" at Caltech.

2019 Completed Harassment and Discrimination Prevention Training at Caltech.

2018, 2016 Lecturer for a 16-day course "Quantum Chemistry" at the "Deutsche SchülerAkademie" for 16 talented pupils.

2015–2016 Lecturer for "Numerical Mathematics for Chemists" (2 hours lecture & 2 hours exercises per week), including a full revision and extension of the lecture notes and exercises.

2013, 2014 Half-day lectures about Analytical Chemistry for pupils participating in the selection rounds of the International Chemistry Olympiad (IChO).

2011 Supervising a research project (awarded) for pupils as STEM mentor ("MINTor") for the Foundation of German Business.

2010, 2011 Preparatory class for first-year Chemistry students.

Professional Service

since 2019 Peer-review for "The Journal of Physical Chemistry Letters," "The Journal of Chemical Physics," "International Journal of Quantum Chemistry" and for "Electronic Structure."

2017 Part of a selection committee for the German Academic Scholarship Foundation ("Studienstiftung").

since 2016 Nomination of four students by letter of recommendation for a fellowship by the German Academic Scholarship Foundation.

2018, 2016 Lecturer for a 16-day course "Quantum Chemistry" at the "Deutsche SchülerAkademie" for 16 talented pupils.

2010–2014 Student representative at the Chemistry department, Kiel University. This included, among others, participation in faculty meetings.

2010–2012 STEM mentor ("MINTor") for the Foundation of German Business encouraging pupils to study a STEM discipline.

since 2009 Work for the Friends of the Chemistry Olympiad, among others organizing and supporting Chemistry contests for pupils.

Publications

12. H. R. Larsson, C. A. Jimenez-Hoyos and G. K.-L. Chan, *Minimal matrix product states and generalizations of mean-field and geminal wavefunctions*, *J. Chem. Theory Comput.*, 16 (2020), 5057–506.

11. H. R. Larsson, *Computing vibrational eigenstates with tree tensor network states (TTNS)*, J. Chem. Phys., 151 (2019), 204102, *Editor's Pick*.

10. H. R. Larsson, J. Riedel, J. Wei, F. Temps and B. Hartke, *Resonance dynamics of DCO ($\widetilde{X}\,^2A'$) simulated with the dynamically pruned discrete variable representation (DP-DVR)*, J. Chem. Phys., 148 (2018), 204309.

9. D. J. Tannor, S. Machnes, E. Assémat and H. R. Larsson, *Phase Space vs. Coordinate Space Methods: Prognosis for Large Quantum Calculations*, Adv. Chem. Phys., 163 (2018), 273-323.

8. D. Azoury, M. Krüger, G. Orenstein, H. R. Larsson, S. Bauch, B. D. Bruner and N. Dudovich, *Self-probing spectroscopy of XUV photo-ionization dynamics in a strong-field environment*, Nature Commun., 8 (2017), 1453.

7. H. R. Larsson and D. J. Tannor, *Dynamical pruning of the multiconfiguration time-dependent Hartree method (DP-MCTDH): An efficient approach for multidimensional quantum dynamics*, J. Chem. Phys., 147 (2017), 044103.

6. H. R. Larsson, B. Hartke and D. J. Tannor, *Efficient molecular quantum dynamics in coordinate and phase space using pruned bases*, J. Chem. Phys., 145 (2016), 204108.

5. S. Machnes, E. Assémat, H. R. Larsson and D. J. Tannor, *Quantum dynamics in phase space using projected von Neumann bases*, J. Phys. Chem. A, 120 (2016), 3296–3308.

4. H. R. Larsson, S. Bauch, L. K. Sørensen and M. Bonitz, *Correlation effects in strong-field ionization of heteronuclear diatomic molecules*, Phys. Rev. A, 93 (2016), 013426.

3. S. Bauch, H. R. Larsson, C. Hinz and M. Bonitz, *The time-dependent generalized active space configuration interaction approach to correlated ionization dynamics of diatomic molecules*, J. Phys. Conf. Ser., 969 (2016), 012008.

2. H. R. Larsson, A. C. T. van Duin and B. Hartke, *Global optimization of parameters in the reactive force field ReaxFF for SiOH*, J. Comput. Chem, 34 (2013), 2178-2189.

1. H. R. Larsson and B. Hartke, *Fitting reactive force fields using genetic algorithms*, Comput. Meth. Mater. Sci., 13 (2013), 120.

Publications in Preparation/under Review

3. H. R. Larsson, H. Zhai and G. K.-L. Chan, *Uncontracted multireference configuration interaction using the density matrix renormalization group*, in preparation.

2. H. R. Larsson, M.Schröder and O. Vendrell, *State-resolved infrared spectrum calculation of the protonated water dimer*, in preparation.

1. H. R. Larsson and D. J. Tannor, *Control of concerted back-to-back double ionization dynamics in helium*, arXiv:2005.10880 (2020).

Awards, Scholarships and Third-Party Funds

2019	Best poster award at the SoCalTheoChem conference, Los Angeles, USA.
2018	Postdoctoral Scholarship by the German Research Foundation (DFG).
2018	Evonik prize for the best Chemistry dissertation of 2018.
2018	Travel grant by the German Academic Exchange Service (DAAD).
2017	Best poster award at the 11th Congress of the World Association of Theoretical and Computational Chemists (WATOC).
2017	Paul Barbara Scholarship for visiting a conference at the Telluride Science Research Center.
2015–2017	PhD Scholarship by the German Academic Scholarship Foundation ("Studienstiftung").
2015–2017	PhD Scholarship by the Chemical Industry Fund (FCI).
2015	Scholarship for studying abroad by the German Academic Exchange Service.
2009–2014	Scholarship by the German Academic Scholarship Foundation.
2014	Otto-Diels-Prize for the best Master's thesis by the Chemistry Department at Kiel University.
2014	Annual prize by the Association for the Support of the Faculty of Mathematics and Natural Sciences at Kiel University.
2014	Award for studies and social commitment by the "Iuventus Academia Holsatorium."
2014	Conference grant by the Society of German Chemists (GDCh).
2013	Invitation to the Lindau Nobel Laureate Meeting, supported by the Chemical Industry Fund.
2012/2013	Erasmus Mobility Grant.
2012	Prize for the Bachelor's thesis by the Chemistry Department at Kiel University.
2009	Award for the best school-leaving examination in Chemistry by the German Chemical Society (GDCh).

Invited Conference Talks

Jul. 2022	Conference "High Dimensional Quantum Dynamics," Groningen, the Netherlands.
Aug. 2021	IUPAC/Canadian Chemistry Conference, Montreal, Canada.
Jun. 2019	Workshop "Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems," Telluride, USA.

Apr. 2019 Workshop "Mathematical Methods in Quantum Molecular Dynamics," Mathematisches Forschungsinstitut Oberwolfach, Germany.

Oct. 2017 Two invited talks at the school "Quantum Dynamics with the Multi-Configuration Time-Dependent Hartree (MCTDH) method: future and perspectives," Orsay, France.

Jul. 2017 Workshop "Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems," Telluride, USA.

Apr. 2017 Annual Meeting of the American Chemical Society, San Francisco, USA (stand-in for D. J. Tannor).

Invited Seminar Talks

Mar. 2021 Group of Prof. A. Bande, Helmholtz Center for Materials and Energy, Berlin, Germany.

Mar. 2021 Physics Seminar, University of Connecticut, Mansfield, USA.

Jan. 2021 Chemistry Seminar, University of California, Los Angeles, USA.

Jan. 2021 Chemistry Seminar, Texas A&M University, College Station, USA.

Jan. 2021 Chemistry Seminar, Auburn University, Auburn, USA.

Dec. 2020 Chemistry Seminar, KTH Royal Institute of Technology, Stockholm, Sweden.

Dec. 2020 Chemistry Seminar, Wayne State University, Detroit, USA.

Oct. 2020 Gas Phase Chemical Kinetics Seminar, Sandia National Laboratories, Livermore, USA.

May. 2020 Chemistry and Chemical Biology Seminar, University of California, Merced, USA.

Nov. 2019 Theoretical Chemistry Seminar, Yale University, New Haven, USA.

Apr. 2019 Theoretical Chemistry Seminar, Ruhr University Bochum, Germany.

Dec. 2018 Christmas Colloquium, Chemistry Department, Kiel Univ., Germany.

Jul. 2018 Group of Prof. P. Schmelcher, Institute of Laser Physics, Hamburg University, Germany.

Jan. 2018 Group of Prof. G. K.-L. Chan, Caltech, Pasadena, USA.

Jan. 2018 Group of Prof. A. I. Krylov, University of Southern California, Los Angeles, USA.

Jan. 2018 Group of Prof. E. Neuscamman, University of California, Berkeley, USA.

Nov. 2017 Theoretical Chemistry Seminar, Heidelberg University, Germany.

Nov. 2016 Group of Prof. I. Burghardt, Goethe University Frankfurt, Germany.

Apr. 2016 Group of Prof. U. Manthe, Bielefeld University, Germany.

Mar. 2016 Group of Prof. I. Burghardt, Goethe University Frankfurt, Germany.

Dec. 2015 Christmas Colloquium, Chemistry Department, Kiel Univ., Germany.

Contributed Talks

Mar. 2021 APS March Meeting, USA.

Aug. 2018 Conference "High Dimensional Quantum Dynamics," Lille, France.

Apr. 2018 Workshop "Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments" at the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

Aug. 2016 Conference "High Dimensional Quantum Dynamics," Rostock, Germany.

Jan. 2016 Workshop of the Friends of the Chemistry Olympiad, Heidelberg, Germany

Oct. 2015 "Advanced Study Group 2015: Semiclassical Methods: Insight and Practice in 'Many' Dimensions," Dresden, Germany.

Dec. 2015 FCI PhD scholar meeting, Braunschweig, Germany.

Apr. 2015 PhD scholar meeting of the German Academic Scholarship Foundation, Berlin, Germany.

Jan. 2013 Workshop of the Friends of the Chemistry Olympiad, Aachen, Germany

Posters

Jul. 2020 Virtual Conference on Theoretical Chemistry, USA.

Feb. 2020 "60th Sanibel Symposium," St. Simons Island, USA.

Jul. 2019 "10th Triennial Congress of the International Society for Theoretical Chemical Physics," Tromsø, Norway.

May. 2019 Awarded poster at the SoCalTheoChem conference, Los Angeles, USA.

Apr. 2018 Workshop "Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments" at the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

Aug. 2017 Awarded poster at the WATOC conference, Munich, Germany.

Jan. 2017 Two posters at the workshop "From Ultrafast to Ultraslow Dynamics in Molecules and Clusters," Rehovot, Israel.

Oct. 2016 Summer school "Modern Wavefunction Methods in Electronic Structure Theory," Gelsenkirchen, Germany.

Sep. 2016 Conference "Quantum Dynamics," Greifswald, Germany.

Sep. 2015 Symposium on Theoretical Chemistry, Potsdam, Germany.

Jun. 2015 CECAM workshop "Molecular Quantum Dynamics Methods," Lausanne, Switzerland.

Dec. 2014 Workshop "Coherence and Control in the Quantum World," Rehovot, Israel.

Sep. 2014 Symposium on Theoretical Chemistry, Vienna, Austria.

Jul. 2014 Sostrup Summer School "Quantum Chemistry and Molecular Properties," Vesterled, Denmark.

Languages

German Native

English Fluent

Swedish Fluent

Hebrew Beginner

Programming Languages and IT

C++17 $>$ 50,000 lines of code

Python 3 $>$ 60,000 lines of code

Fortran 95 $>$ 50,000 lines of code

Matlab $>$ 5,000 lines of code

(Arch) Linux $>$ 10 years experience

Interests

- Running
- Hiking
- Skiing
- Cooking
- Philosophy (Epistemology, Constructivism)