

Henrik R. Larsson

Curriculum Vitae

University of California, Merced
Department of Chemistry & Biochemistry
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Theoretical Chemist

Professional Experience

- since Apr. 2022 **Assistant Professor of Chemistry**, *University of California, Merced, USA*, affiliate position in Physics.
- Sept 2018–Mar. 2022 **Postdoctoral Scholar Research Associate**, *California Institute of Technology, USA*.
- Dec. 2014–Sept 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 the density matrix renormalization group (DMRG) in order to efficiently simulate strongly correlated quantum systems. Connections between the DMRG and simple methods such as valence bond are explored. Development of DMRG-based multireference coupled cluster methods. Development of DMRG-based method that improves vibrational spectra simulations of fluxional molecules by orders of magnitudes.

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)
- Two stays at Weizmann Institute: 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 (machine learning technique). 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

- Referee The Journal of Physical Chemistry Letters, Journal of Chemical Theory and Computation, The Journal of Chemical Physics, Physical Chemistry Chemical Physics, International Journal of Quantum Chemistry, Electronic Structure, International journal of Chemical Kinetics, Journal of Physics: Condensed Matter.
- 2017 Member of the selection committee for the German Academic Scholarship Foundation ("Studienstiftung").
- since 2016 Nomination of four students by letter of recommendation for a fellowship from 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, active 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

16. **H. R. Larsson**, M. Schröder, R. Beckmann, F. Briec, C. Schran, D. Marx, and O. Vendrell, *State-resolved infrared spectrum calculation of the protonated water dimer*, Chem. Sci., Edge Article, in press.
15. **H. R. Larsson**, H. Zhai, C. J. Umrigar and G. K.-L. Chan, *The chromium dimer: closing a chapter of quantum chemistry*, J. Am. Chem. Soc. Communication, 144 (2022), 15932-15937.
14. **H. R. Larsson**, H. Zhai, K. Gunst and G. K.-L. Chan, *Matrix product states with large sites*, J. Chem. Theory Comput., 18 (2022), 749-762.
13. **H. R. Larsson** and D. J. Tannor, *Control of concerted back-to-back double ionization dynamics in helium*, J. Chem. Phys., 155 (2021), 144105.
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 (\tilde{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.

Awards, Scholarships and Third-Party Funds

- 2019 US Junior Oberwolfach Fellow
- 2019 Best poster award at the SoCalTheoChem conference, Los Angeles, USA.
- 2018 Postdoctoral Scholarship from the German Research Foundation (DFG).
- 2018 Evonik prize for the best Chemistry dissertation of 2018.
- 2018 Travel grant from 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 from the Telluride Science Research Center.
- 2015–2018 PhD Scholarship from the German Academic Scholarship Foundation (“Studiens-tiftung”).
- 2015–2017 PhD Scholarship from the Chemical Industry Fund (FCI).
 - 2015 Scholarship for studying abroad from the German Academic Exchange Service.
- 2009–2014 Scholarship from the German Academic Scholarship Foundation.
 - 2014 Otto-Diels-Prize for the best Master’s thesis from the Chemistry Department at Kiel University.
 - 2014 Annual prize from the Association for the Support of the Faculty of Mathematics and Natural Sciences at Kiel University.
 - 2014 Award for studies and social commitment from the “Iuventus Academia Holsatorium.”
 - 2014 Conference grant from 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 Bachelor’s Thesis Prize from the Chemistry Department at Kiel University.
 - 2009 Award for the best school-leaving examination in Chemistry from the German Chemical Society (GDCh).

Invited Conference Talks

- June 2023 “Strong Correlation in Molecules” satellite symposium of the ICQC congress, Znojmo, Czech Republic.

- Sept. 2022 "Symposium for Theoretical Chemistry," Heidelberg, Germany.
- Jul. 2022 "High Dimensional Quantum Dynamics" conference, Groningen, the Netherlands.
- Jun. 2022 "Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems" workshop, Telluride, USA.
- Sep. 2021 Quantum dynamics network meeting, Paris, France.
- Aug. 2021 IUPAC/Canadian Chemistry Conference, Montreal, Canada.
- Jun. 2019 "Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems" workshop, Telluride, USA.
- Apr. 2019 "Mathematical Methods in Quantum Molecular Dynamics" workshop, Mathematisches Forschungsinstitut Oberwolfach, Germany.
- Oct. 2017 Two invited talks at "Quantum Dynamics with the Multi-Configuration Time-Dependent Hartree (MCTDH) method: future and perspectives" International School, Paris-Saclay University, Orsay, France.
- Jul. 2017 "Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems" workshop, Telluride, USA.
- Apr. 2017 American Chemical Society Annual Meeting, San Francisco, USA (stand-in for D. J. Tannor).

Invited Seminar Talks

- May. 2022 Theoretical Chemistry Seminar, University of Tübingen, Germany.
- Dec. 2021 Prof. S. De Baerdemacker Group, University of New Brunswick, Fredericton, Canada
- Jun. 2021 Chemistry Seminar, University of California, Merced, USA.
- Jun. 2021 Principal Investigator Fellowship Symposium, RWTH Aachen University, Germany.
- May 2021 Chemistry Seminar, Technical University of Munich, Germany.
- Mar. 2021 Prof. A. Bande Group, Helmholtz Center for Materials and Energy, Berlin, Germany.
- Mar. 2021 Physics Seminar, University of Connecticut, Mansfield, USA.
- Feb. 2021 Chemistry Seminar, University of California, Davis, 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 Prof. P. Schmelcher Group, Institute of Laser Physics, Hamburg University, Germany.
- Jan. 2018 Prof. G. K.-L. Chan Group, Caltech, Pasadena, USA.
- Jan. 2018 Prof. A. I. Krylov Group, University of Southern California, Los Angeles, USA.
- Jan. 2018 Prof. E. Neuscammann Group, University of California, Berkeley, USA.
- Nov. 2017 Theoretical Chemistry Seminar, Heidelberg University, Germany.
- Nov. 2016 Prof. I. Burghardt Group, Goethe University Frankfurt, Germany.
- Apr. 2016 Prof. U. Manthe Group, Bielefeld University, Germany.

- Mar. 2016 Prof. I. Burghardt Group, Goethe University Frankfurt, Germany.
Dec. 2015 Christmas Colloquium, Chemistry Department, Kiel Univ., Germany.

Contributed Talks

- Mar. 2021 American Physical Society March Meeting, USA.
Aug. 2018 "High Dimensional Quantum Dynamics" conference, Lille, France.
Apr. 2018 "Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments" workshop at the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.
Aug. 2016 "High Dimensional Quantum Dynamics" conference, Rostock, Germany.
Jan. 2016 Friends of the Chemistry Olympiad Workshop, Heidelberg, Germany
Oct. 2015 "Advanced Study Group 2015: Semiclassical Methods: Insight and Practice in 'Many' Dimensions" workshop, Dresden, Germany.
Dec. 2015 FCI PhD scholar meeting, Braunschweig, Germany.
Apr. 2015 German Academic Scholarship Foundation PhD scholar meeting, Berlin, Germany.
Jan. 2013 Friends of the Chemistry Olympiad Workshop, Aachen, Germany

Posters

- Mar. 2021 "Tensor product methods for strongly correlated molecular systems" workshop, MPIPKS Dresden, Germany.
Mar. 2021 American Physical Society March Meeting, USA.
Jul. 2020 Virtual Conference on Theoretical Chemistry, USA.
Feb. 2020 "60th Sanibel Symposium" conference, St. Simons Island, USA.
Jul. 2019 "10th Triennial Congress of the International Society for Theoretical Chemical Physics" conference, Tromsø, Norway.
May 2019 SoCalTheoChem conference, Los Angeles, USA. (*Best Poster Award*)
Apr. 2018 "Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments" workshop at the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.
Aug. 2017 WATOC conference, Munich, Germany. (*Best Poster Award*)
Jan. 2017 Two posters at the "From Ultrafast to Ultraslow Dynamics in Molecules and Clusters" workshop, Rehovot, Israel.
Oct. 2016 "Modern Wavefunction Methods in Electronic Structure Theory" summer school, Gelsenkirchen, Germany.
Sep. 2016 "Quantum Dynamics" conference, Greifswald, Germany.
Sep. 2015 Symposium on Theoretical Chemistry, Potsdam, Germany.
Jun. 2015 CECAM "Molecular Quantum Dynamics Methods" workshop, Lausanne, Switzerland.
Dec. 2014 "Coherence and Control in the Quantum World" conference, Rehovot, Israel.
Sep. 2014 Symposium on Theoretical Chemistry, Vienna, Austria.
Jul. 2014 "Quantum Chemistry and Molecular Properties" Sostrup Summer School, Vesterled, Denmark.