Henrik R. Larsson

Curriculum Vitae

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

Research Interests

Molecular Quantum Dynamics, Electronic Structure Theory, Electron Dynamics, Tensor Network Methods, Quantum Control Theory

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.

Awards, Scholarships and Third-Party Funds

2023 "State-resolved vibrational spectra of fluxional protonated water clusters via tensor network states", National Science Foundation: $514,668.

2023 "Advancing Atomistic Understanding of Electronic Energy Transfer", Department of Energy: $630,000; Larsson is co-PI; ∼ $200,000 to Larsson.

2022 "Unraveling Attosecond Molecular Charge Migration by Quantum Dynamics Simulations using Novel Quantum Simulation Tools", UC Merced Senate Faculty Research Grant: $7,380.

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 ("Studienstiftung").
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	Kiel University's most renowned Holstein Study 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).

Professional Service and Outreach

Review Panel Member	Naional Science Foundation
Article Reviewer	The Journal of Physical Chemistry Letters, Journal of Chemical Theory and Computation, The Journal of Chemical Physics, Physical Chemistry Chemical Physics, Molecular Physics, Journal of Physics Communications, International Journal of Quantum Chemistry, Electronic Structure, International Journal of Chemical Kinetics, Journal of Physics: Condensed Matter, Quantum Science and Technology.
2024	Scientific co-organizer of "Recent progress on tensor network methods" workshop at TUM Institute for Advanced Study.
2024	Scientific co-organizer of "West Coast Theoretical Chemistry Meeting" at UC Merced.
2023,2024	Scientific committee member of High Dimensional Quantum Dynamics conference.
2023	Scientific organizer of a Quantum Dynamics Workshop, Wolfgang Pauli Institute, Vienna.
2023	Lecturer at Quantum Dynamics Network MCTDH Summer School, IWR Heidelberg.
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.

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

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

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

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

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

Publications

Book Chapters (peer-reviewed)

1. 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.

Journal Articles (peer-reviewed)

17. **H. R. Larsson**, *A tensor network view of multilayer multiconfiguration time-dependent Hartree methods*, Mol. Phys., e2306881 (2024), **invited New View Article**.

16. H. Zhai, **H. R. Larsson**, et al., *Block2: a comprehensive open source framework to develop and apply state-of-the-art DMRG algorithms in electronic structure and beyond*, J. Chem. Phys. , 159 (2023), 234801.

15. **H. R. Larsson**, M. Schröder, R. Beckmann, F. Brieuc, C. Schran, D. Marx, and O. Vendrell, *State-resolved infrared spectrum calculation of the protonated water dimer*, Chem. Sci., Edge Article, 13 (2022), 11119-11125.

14. **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.

13. **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.

12. **H. R. Larsson** and D. J. Tannor, *Control of concerted back-to-back double ionization dynamics in helium*, J. Chem. Phys., 155 (2021), 144105.

11. **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.

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

9. **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.

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 under Review

Invited Conference Talks

Jun. 2024	"Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems" workshop, Telluride, USA.
Apr. 2024	"Recent progress on tensor network methods" workshop, Munich, Germany.
Apr. 2024	4th "Atoms, Molecules and Clusters in Motion" conference, Paris, France.
Jul. 2023	"Tensor Network Methods in Quantum Dynamics" workshop, Wolfgang Pauli Institute Vienna, Austria.
Jun. 2023	35th Workshop on Recent Developments in Electronic Structure Methods, Merced, USA.
Jun. 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

Oct. 2022	Physics Seminar, University of California, Merced, USA.
Sep. 2022	Prof. P. Schmelcher Group, Institute of Laser Physics, Hamburg University, Germany.
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. Neuscamman 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

Aug. 2023	American Chemical Society Annual Meeting, San Francisco, USA.
May. 2023	West Coast Theoretical Chemistry Meeting, Davis USA.
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

May. 2023 West Coast Theoretical Chemistry meeting, USA.

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.