

HEATHER WIEBE

Curriculum Vitae

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Current Position

Assistant Professor Nov. 2020 -
Department of Chemistry, Vancouver Island University

Adjunct Professor Nov. 2021 -
Department of Chemistry, University of Victoria

Education

Ph.D. in chemistry 2018
Simon Fraser University, Canada
Supervisors: Noham Weinberg and Michael Eikerling
Thesis: Mechanistic applications of volume profiles for chemical and biochemical processes.

B.Sc. in chemistry (major) and biology (minor) 2011
University of the Fraser Valley, Canada
Dean's Medal of Excellence, GPA: 4.10

Postdoctoral Experience

Postdoctoral Research Associate May 2018 – Sept. 2020
School of Physics & Astronomy, University of Edinburgh
Supervisor: Graeme Ackland
Project: Nuclear quantum effects in compressed materials via path integral molecular dynamics

Publications

1. Underwood, T., **Wiebe, H.** and Ackland, G. J. "A method for pinpointing solid-solid phase transitions in quantum crystals: Application to solid hydrogen" *In preparation for the Journal of Chemical Physics*.
2. van de Bund, S., **Wiebe, H.** and Ackland, G. J. "Isotope quantum effects in the metallization transition to liquid hydrogen" *Physical Review Letters* **126**, 225701 (2021)
3. **Wiebe, H.**, Underwood, T. and Ackland, G. J. "Phase behaviour of the quantum Lennard-Jones solid" *Journal of Chemical Physics* **153**, 074502 (2020)
4. Zong, H., **Wiebe, H.** and Ackland, G. J. "Understanding high pressure hydrogen with a hierarchical machine-learned potential" *Nature Communications* **11**, 5014 (2020)

5. Spooner, J., **Wiebe, H.**, Louwarse, M., Reader, B. and Weinberg, N. "Theoretical analysis of high pressure effects on conformational equilibria." *Canadian Journal of Chemistry* **96**, 178-189 (2018).
6. **Wiebe, H.**, Louwarse, M. and Weinberg, N. "Theoretical volume profiles for conformational changes: Application to internal rotation of benzene ring in 1,12-dimethoxy-[12]-paracyclophane." *Journal of Chemical Physics* **146**, 104107 (2017).
7. **Wiebe, H.**, Louwersheimer, J. and Weinberg, N. "Molecular dynamic studies of the solubility of sodium chloride: Fast calculations using seed crystalline cluster probe." *Molecular Physics* **113**, 1-6 (2015).
8. **Wiebe, H.** and Weinberg, N. "Theoretical volume profiles as a tool for probing transition states: folding kinetics." *Journal of Chemical Physics* **140**, 124105 (2014)
9. **Wiebe, H.**, Prachnau, M. and Weinberg, N. "Hydrogen transfer reactions in viscous media: potential and free energy surfaces in solvent-solute coordinates and their kinetic implications." *Canadian Journal of Chemistry* **91**, 787-794 (2013).
10. **Wiebe, H.**, Spooner, J., Boon, N., Deglint, E., Edwards, E., Dance, P. and Weinberg, N. "Calculation of molecular volumes and volumes of activation via molecular dynamics simulations." *Journal of Physical Chemistry C* **116**, 2240–2245 (2012).
11. Spooner, J., **Wiebe, H.**, Boon, N., Deglint, E., Edwards, E., Yanciw, B., Patton, B., Thiele, L., Dance P. and N. Weinberg. "Molecular dynamics calculation of molecular volumes and volumes of activation." *Physical Chemistry Chemical Physics* **14**, 2264-2277 (2012).
12. Deglint, E., **Wiebe, H.**, Edwards, E., Boon, N., Dance, P. and Weinberg, N. "Molecular dynamics calculation of activation volumes." *Physical Chemistry Chemical Physics* **13**, 438-440 (2011).

Grants and Funding

Discovery Grant (\$120,000 CAD)	2021 – 2026
Discovery Grant Early Career Launch Supplement (\$12,500 CAD) Natural Sciences and Research Council of Canada Title: <i>Under the sea: The effect of high pressure on marine biochemistry</i>	
VIU Research Council Explore Grant (\$2000 CAD)	2021 – 2022
VIU Research Council Inquiry Grant (\$5000 CAD) Vancouver Island University Title: <i>How do amino acid substitutions confer pressure-resistance in deep-sea fish?</i>	
Undergraduate Research Assistant Positions Canada Summer Jobs Program (\$3192 CAD) VIU Work-Op Program (\$1520 CAD)	2021
Scottish Academic Compute Allocation Edinburgh Parallel Computing Centre	2019 – 2020

Title: <i>Nuclear quantum effects in hydrogen and deuterium from path integral molecular dynamics</i>	
Professional Development Grant (\$499 CAD) Simon Fraser University Graduate Student Society	2017
Graduate fellowship (\$7000 CAD) Simon Fraser University Chemistry Department	2016 & 2013
Alexander Graham Bell CGS – Doctoral Level (\$105,000 CAD) Natural Sciences and Research Council of Canada Title: <i>Towards a volumetric method for identification and characterization of the transition state ensemble for conformational changes in macromolecules</i>	2013 – 2016
Alexander Graham Bell CGS - Master's level (\$17,500 CAD) Natural Sciences and Research Council of Canada Title: <i>Characterization of the transition state ensemble for protein folding using molecular dynamics calculations of molecular volumes</i>	2011 – 2012

Selected Honours and Awards

Hans Neurath Outstanding Promise Travel Award (\$2000 USD) The Protein Society	2015
ACS Chemical Computing Group Research Excellence Award (\$1150 USD) American Chemical Society & Chemical Computing Group	2014
Travel Award from Oral Presentation Competition (\$1000 CAD) Simon Fraser University Chemistry Department	2013
Outstanding Poster Award (\$50 CAD) Canadian Symposium on Theoretical and Computational Chemistry	2012 & 2010
Provost's Prize of Distinction (\$5000 CAD) Simon Fraser University Office of Graduate Studies	2011
Outstanding Achievement by a Student Graduating with a Chemistry Major University of the Fraser Valley Chemistry Department	2011
Dean's Medal of Excellence University of the Fraser Valley Faculty of Science	2011
Industry Liaison Research Award (\$1000 CAD) University of the Fraser Valley Research Office	2011
Undergraduate Student Research Award (\$4500 CAD) Natural Science and Research Council of Canada	2011 & 2009

Research Excellence Award (\$500 CAD) University of the Fraser Valley Research Office	2009
Silver Medal (\$50 CAD) Canadian Society for Chemistry	2009
Dean of Science Poster Award (\$75 CAD) University of the Fraser Valley Faculty of Science	2009

Supervisory Experience

Ph.D. students (co-supervisor)

University of Edinburgh

Sebastiaan van de Bund Thesis: <i>Nuclear quantum effects in compressed hydrogen and deuterium</i>	2019 – present
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Undergraduate students (primary investigator)

Vancouver Island University

Mark Bracken Project: <i>Catalytic activity of lactate dehydrogenase at high pressure from QM/MM simulations</i>	2021
Savannah Mercer Project: <i>The effect of amino acid substitution on the thermodynamic stability of lactate dehydrogenase at high pressure</i>	2021
Diego Franco Project: <i>Fragmentation patterns in prostaglandins from first principles</i>	2021
Jocelyn Maguire Jordan Davis Project: <i>The effect of amino acid substitution on the volume change of unfolding in pressure-resistant lactate dehydrogenase</i>	2021 2021
Emily Mahony Project: <i>The effect of trimethylamine-N-oxide on the dissociation of the lactate dehydrogenase tetramer complex</i>	2021

Undergraduate students (co-supervisor)

University of Edinburgh

Angus Gentles Maxim Oweyssi Project: <i>Pressure dependence of the vibron frequency of solid hydrogen from first principles</i>	2020 2020
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Althea Lai	2019
Project: <i>Nuclear quantum effects from path integral molecular dynamics</i>	
Balagardash Bashirov	2019
Vedant Bhargava	2019
Project: <i>Probing the liquid-liquid phase transition in hydrogen and deuterium</i>	
<u>University of the Fraser Valley</u>	
Miranda Louwerse	2015 – 2017
Project: <i>Pressure controlled molecular machines</i>	
Abigail Sherwood	2016 – 2017
Project: <i>The effect of high pressure on radical hydrogen abstraction</i>	
Kelsy Yeung	2015
Project: <i>Theoretical study of fluorescent properties of tryptophan in staphylococcal nuclease unfolding</i>	
Brandon Wiebe	2015
Project: <i>Complexation volumes of crown ethers</i>	
Hars Virk	2014
Project: <i>The effect of pressure on conformational volumes</i>	
Karanjit Singh	2013
Project: <i>Prediction of solubility of ionic compounds from molecular dynamics simulations</i>	

Conference Presentations

Oral Presentations

Wiebe, H., Zong, H. and Ackland, G. J. “Nuclear quantum effects in compressed hydrogen and deuterium from path integral molecular dynamics” 57th EHPG Meeting on High Pressure Science and Technology, September 2019, Prague, Czech Republic.

Wiebe, H. and Weinberg, N. “Volume profiles for conformational changes in macromolecules and their mechanistic applications” Pacifichem, December 2015, Honolulu, Hawaii.

Wiebe, H. and Weinberg, N. “Volume profiles for conformational changes in flexible systems and their mechanistic applications” AIRAPT-25/EHPG-53 International Conference on High Pressure Science and Technology, September 2015, Madrid, Spain.

Wiebe, H. and Weinberg, N. “Volume profiles as a tool for probing the transition states of protein folding” 97th Canadian Chemistry Conference and Exhibition, June 2014, Vancouver.

Wiebe, H. and Weinberg, N. “Volume profiles as a tool for probing the transition states of protein folding” Frontiers in Biophysics, March 2014, Simon Fraser University.

Wiebe, H. and Weinberg, N. "Identification of transition state ensembles using MD-calculated volume profiles and volumes of activation." Annual Oral Presentation Competition, January 2013, Department of Chemistry, Simon Fraser University.

Wiebe, H. and Weinberg N. "Research group as a community of learners: Two viewpoints on its internal and external dynamics." Invited speaker, Academic conference: *Is there an R in Teaching? Is there a T in Research?*, May 2011, University of the Fraser Valley.

Wiebe, H. "Characterization of the transition state ensemble for protein folding using molecular dynamics calculations of molecular volumes" Microlecture series, March 2011, University of the Fraser Valley.

Wiebe, H. and Prachnau, M. "High pressures around the world: The effect of viscosity on the pyrolysis of *n*-octane." Invited speaker, NSERC lecture series, November 2010, University of the Fraser Valley.

Poster Presentations

Wiebe, H., Sherwood, A., Spooner, J. and Weinberg, N. "The effect of elevated pressure on radical hydrogen abstraction" 100th Canadian Chemistry Conference and Exhibition, May 2017, Toronto.

Wiebe, H., Louwerse, M. and Weinberg, N. "Pressure-controlled conformational tuning in molecular wires and rotors" 100th Canadian Chemistry Conference and Exhibition, May 2017, Toronto.

Wiebe, H. and Weinberg, N. "Theoretical volume profiles as a tool for probing the protein folding transition state ensemble" The 19th Annual Symposium of the Protein Society, July 2015, Barcelona, Spain.

Wiebe, H. and Weinberg, N. "MD-generated volume profiles as a tool for probing transition states of conformational changes" 249th ACS National Meeting & Exhibition, March 2015, Denver, Colorado.

Wiebe, H. and Weinberg, N. "Probing protein folding using MD-generated volume profiles and experimental volumes of activation" 51st International Meeting of the European High Pressure Research Group, September 2013, London, England.

Wiebe, H. Spooner, J. and Weinberg, N. "Identification of TS structures by a combination of high pressure kinetics and MD volume calculations" 24th Biennial International Conference of the International Association for the Advancement of High Pressure Science and Technology, July 2013, Seattle.

Wiebe, H. and Weinberg, N. "Probing protein folding with high pressure MD simulations" 96th Canadian Chemistry Conference and Exhibition, May 2013, Québec.

Wiebe, H. and Weinberg, N. "MD-generated volume profiles for study of the folding of macromolecules" Frontiers in Biophysics Conference, March 2013, University of British Columbia.

Wiebe, H. and Weinberg, N. "MD-generated volume profiles for study of conformational changes in macromolecules" 13th Annual Chemistry Graduate Student Poster Competition, November 2012, Simon Fraser University.

Wiebe, H., Spooner, J. and Weinberg, N. "Method for identification of transition states using MD-generated volume profiles and volumes of activation" 25th Canadian Symposium on Theoretical and Computational Chemistry, July 2012, University of Guelph.

Wiebe, H. and Weinberg, N. "MD-generated volume profiles for study of the folding of macromolecules" 95th Canadian Chemistry Conference and Exhibition, May 2012, Calgary.

Wiebe, H., Epp, A., Wong, W., Prachnau, M. Perkins, J. Fenske, D. and Weinberg, N. "Technique for the regeneration of petroleum-contaminated vegetable oil" Undergraduate Research Day, March 2011, University of the Fraser Valley.

Boon, N., Deglint, E., Edwards, E., **Wiebe, H.,** Dance, P. and Weinberg, N. "Calculation of molecular volumes using molecular dynamics simulations: activation and reaction volumes." 17th Canadian Symposium on Theoretical Chemistry, August 2010, University of Alberta.

Wiebe, H. and Weinberg, N. "The effect of pressure on hydrogen transfer between simple hydrocarbon species" Undergraduate Research Day, March 2010, University of the Fraser Valley.

Wiebe, H., Prachnau, M. and Weinberg, N. "The effect of pressure on the rates of hydrogen transfer in simple hydrocarbon species." Undergraduate Research Day, March 2009, University of the Fraser Valley.

Service & Professional Involvement

Society memberships

Canadian Association of Theoretical Chemists	2021 – Present
European High Pressure Research Group	2015 – Present
International Association for the Advancement of High-Pressure Science and Technology	2015 – Present

Other professional activities

Member of MPhys marking panel (University of Edinburgh)	2019 – 2020
Organizer for computational material physics seminars (University of Edinburgh)	2018 – 2020
Social Coordinator for the SFU Chemistry Graduate Caucus (Simon Fraser University)	2013 – 2015
Team leader on an NSERC Engage Grant project (University of the Fraser Valley)	2010 – 2011
Organizer, Undergraduate Science Research Night (University of the Fraser Valley)	2009