Johannes Hachmann, PhD — Curriculum Vitae

University at Buffalo, The State University of New York
Department of Chemical and Biological Engineering
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PROFESSIONAL BACKGROUND

- **Assistant Professor**, Department of Chemical and Biological Engineering (CBE) — since 2014
- **Faculty Member**, New York State Center of Excellence in Materials Informatics (CMI) — since 2014
- **Core Faculty Member**, Computational and Data-Enabled Science and Engineering Program (CDSE) — since 2014
- **Faculty Member**, Institute for Research and Education in eNergy, Environment, and Water (RENEW) — since 2015
  University at Buffalo, The State University of New York (Buffalo, NY)

- **Research Associate** — 2012 – 2014
- **Postdoctoral Research Fellow** — 2009 – 2012
  Harvard University (Cambridge, MA), Department of Chemistry and Chemical Biology
  Advisor: Prof. Alán Aspuru-Guzik

- **Graduate Research and Teaching Assistant** — 2004 – 2009
  Cornell University (Ithaca, NY), Department of Chemistry and Chemical Biology
  Advisor: Prof. Garnet K.-L. Chan

- **Undergraduate Research Assistant** — 2003 – 2004
  University of Cambridge (UK), Department of Chemistry
  Advisor: Prof. Nicholas C. Handy†

EDUCATION

- **PhD**, Theoretical Chemistry, Feb 2010
  Ab initio density matrix renormalization group methodology and computational transition metal chemistry
- **MSc**, Theoretical Chemistry, Jan 2007
  Development of density matrix renormalization group methodology in electronic structure theory
  Cornell University, Department of Chemistry and Chemical Biology — 2004 – 2009
  Advisor: Prof. Garnet K.-L. Chan

- **DiplChem**, Theoretical Chemistry, Dec 2004
  Nodal hypersurfaces and sign domains in many-electron wavefunctions
- **Predipl**, Chemistry, Oct 2001
  University of Jena (Germany), School of Chemistry and Earth Sciences — 1999 – 2004
  University of Cambridge (UK), Department of Chemistry — 2003 – 2004
  Advisors: PD Dr. Hans-Gerhardt Fritsche, Prof. Nicholas C. Handy†

AWARDS & HONORS

- Finalist of the Emerging Technologies in Computational Chemistry Competition of the ACS Division of Computers in Chemistry — 2016
- Runner-Up Professor of the Year of the AIChE Buffalo Student Chapter — 2016
- Computerworld Data+ Award (with the Clean Energy Project team) — 2013
- RSC Scholarship Award for Scientific Excellence of the ACS Division of Chemical Information — 2013
- ACS Division of Physical Chemistry Postdoctoral Research Award — 2013
- IBM-Löwdin Award — 2013

AWARDS & HONORS (CONTINUED)

- International Congress of Quantum Chemistry Outstanding Poster Award 2012
- Finalist of the CycleCloud BigScience Challenge with Honorable Mention 2011
- CSC Best Poster Presentation Award of the Physical, Theoretical and Computational Division 2009
- APS Graduate Student Travel Award of the Division of Chemical Physics 2008
- IBM-Zerner Fellowship Award 2008
- Strongly Correlated Electron Systems Young Investigator Award 2007
- CCG Excellence Award of the ACS Division for Computers in Chemistry 2006
- Kekulé Fellowship of the Fund of the German Chemical Industry 2005 – 2007
- Diploma with Distinction 2004
- Study-Abroad-Scholarship of the German National Academic Foundation 2003 – 2004
- Scholarship of the German National Academic Foundation 2000 – 2004

GRANTS & FUNDING

- NYS Center of Excellence in Materials Informatics, Collaboration Funding, $25k: 2017 – 2018
  Joining Forces to Develop the Tools and Techniques for Materials Informatics 2.0
- DOD ARO Small Business Innovation Research Program (with Technology Holding LLC), $150k: 2017 – 2018
  Informatics-driven design of eutectics and nanomaterials-based supercapacitors for enhanced low-temperature performance
- NSF CHE Special Projects Program (with T. Windus, J. McLean), $79k: 2017 – 2018
  CHE Workshop: Framing the Role of Big Data and Modern Data Science in Chemistry
- NSF IIS Big Data Spokes (Big Data Regional I) Program (with A. Patra *et al.*), $100k: 2016 – 2017
  BD Spokes: Planning: NORTHEAST: Partnerships for energy-cycle innovation through big data
- NYS Center of Excellence in Materials Informatics, Collaboration Funding (with C. Cheng), $40k: 2015 – 2016
  Development of biodegradable polymers for medical applications guided by materials informatics
- NSF IIS Big Data Regional Innovation Hubs Program (with K. McKeown *et al.*), $1.25M: 2015 – 2018
  BD Hubs: Collaborative Proposal: NORTHEAST: The Northeast Big Data Innovation Hub
- NSF CBET Energy for Sustainability Program (with G. Wu, C. Cheng), $300k: 2015 – 2018
  UNS: 3-dimensional porous nanographene for highly efficient energy storage in Li-ion batteries
- NYS Center of Excellence in Materials Informatics, Seed Funding, $17k: 2015
  UB Solar Fuel Project
- UUP Individual Development Award 2014, 2015
- UB Undergraduate STEM Mentoring and Program Development Award 2014
- CSA Trust Jacques-Émile Dubois Grant (Chemical Structure Association) 2013
- Grant of the President's January Innovation Fund for Faculty 2012
- GAIN Travel Grant (German Academic International Network) 2009, 2012
- ACS Cornell Section Graduate Student Conference Grant 2007
- Cornell Graduate Student Conference Grant 2006, 2007, 2009

PUBLICATIONS

14. R. Asatryan, E. Ruckenstein, **J. Hachmann**, *Revisiting the polytopal rearrangements in penta-coordinate d^7-metallocomplexes: modified Berry pseudorotation, octahedral switch, and butterfly isomerization*, Chem. Sci. 8 (**2017**), 5512-5525.
13. E.O. Pyzer-Knapp, G. Simm, T. Lutzow, K. Li, L.R. Seress, **J. Hachmann**, A. Aspuru-Guzik, *The Harvard Organic Photovoltaic Dataset*, Sci. Data 3 (**2016**), 160086.
12. **J. Hachmann**, R. Olivares-Amaya, A. Jinich, A.L. Appleton, M.A. Blood-Forsythe, L.R. Seress, C. Román-Salgado, K. Trepte, S. Atahan-Evrenk, S. Er, S. Shrestha, R. Mondal, A. Sokolov, Z. Bao, A. Aspuru-Guzik, *Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry – the Harvard Clean Energy Project*, Energy Environ. Sci. 7 (**2014**), 698-704.
11. C. Amador-Bedolla, R. Olivares-Amaya, **J. Hachmann**, A. Aspuru-Guzik, *Organic photovoltaics*, in Informatics for Materials Science and Engineering – Data-driven Discovery for Accelerated Experimentation and Application, K. Rajan, Ed., Elsevier, Amsterdam (**2013**), 423-442.

PUBLICATIONS (CONTINUED)

10. R. Olivares-Amaya, C. Amador-Bedolla, **J. Hachmann**, S. Atahan-Evrenk, R.S. Sánchez-Carrera, L. Vogt, A. Aspuru-Guzik, *Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics*, Energy Environ. Sci. 4 (**2011**), 4849-4861.
9. **J. Hachmann**, R. Olivares-Amaya, S. Atahan-Evrenk, C. Amador-Bedolla, R.S. Sánchez-Carrera, A. Gold-Parker, L. Vogt, A.M. Brockway, A. Aspuru-Guzik, *The Harvard Clean Energy Project: large-scale computational screening and design of organic photovoltaics on the World Community Grid*, J. Phys. Chem. Lett. 2 (**2011**), 2241-2251.
8. **J. Hachmann**, B.A. Frazier, P.T. Wolczanski, G.K.-L. Chan, *A theoretical study of the 3d-M(smif)$_2$ complexes: structure, magnetism, and oxidation states*, ChemPhysChem 12 (**2011**), 3236-3244.
7. J.J. Dorando, **J. Hachmann**, G.K.-L. Chan, *Analytic response theory for the density matrix renormalization group*, J. Chem. Phys. 130 (**2009**), 184111.
6. D. Ghosh, **J. Hachmann**, T. Yanai, G.K.-L. Chan, *Orbital optimization in the density matrix renormalization group, with application to polyenes and β-carotene*, J. Chem. Phys. 128 (**2008**), 144117.
5. G.K.-L. Chan, J.J. Dorando, D. Ghosh, **J. Hachmann**, E. Neuscamman, H. Wang, T. Yanai, *An introduction to the density matrix renormalization group ansatz in quantum chemistry*, Prog. Theor. Chem. Phys. 18 (**2008**), 49-65.
4. **J. Hachmann**, J.J. Dorando, M. Avilés, G.K.-L. Chan, *The radical character of the acenes: A density matrix renormalization group study*, J. Chem. Phys. 127 (**2007**), 134309.
3. J.J. Dorando, **J. Hachmann**, G.K.-L. Chan, *Targeted excited state algorithms*, J. Chem. Phys. 127 (**2007**), 084109.
2. **J. Hachmann**, W. Cardoen, G.K.-L. Chan, *Multireference correlation in long molecules with the quadratic scaling density matrix renormalization group*, J. Chem. Phys. 125 (**2006**), 144101.
1. **J. Hachmann**, P.T.A. Galek, T. Yanai, G.K.-L. Chan, N.C. Handy, *The nodes of Hartree-Fock wavefunctions and their orbitals*, Chem. Phys. Lett. 392 (**2004**), 55-61.

Summary: 1100+ citations; h-index: 10; i10-index: 10

PUBLICATIONS IN PREPARATION

- M.A. Faiz Afzal, C. Cheng, **J. Hachmann**, *Combining first-principles and data modeling for the accurate prediction of the refractive index of organic polymers*, to be submitted to Chem. Mater. (invited).
- M. Haghighatlari, **J. Hachmann**, *Trend-based feature selection in molecular descriptor space*, to be submitted to Mater. Discovery (invited).
- **J. Hachmann**, *A graduate student's guide to writing papers*, to be submitted to Int. J. Quantum Chem. (invited tutorial).
- Y. Tian, M. Haghighatlari, **J. Hachmann**, *Inheritance of molecular orbital energies from monomer building blocks to larger copolymers and implications for the rational design of organic semiconductors*, to be submitted to Mater. Discovery (published as part of the MSc thesis of Y. Tian).
- B.A. Moore, C.-Y. Shih, M. Haghighatlari, **J. Hachmann**, *Systematic trends in results from different DFT model chemistries I: Efficient projection schemes*, to be submitted to Int. J. Quantum Chem. (published as part of the MSc thesis of C.-Y. Shih).
- C.-Y. Shih, M. Haghighatlari, B.A. Moore, **J. Hachmann**, *Systematic trends in results from different DFT model chemistries II: Structural patterns related to non-systematic behavior*, to be submitted to Int. J. Quantum Chem. (published as part of the MSc thesis of C.-Y. Shih).
- C.-Y. Shih, M. Haghighatlari, B.A. Moore, **J. Hachmann**, *Systematic trends in results from different DFT model chemistries III: Machine learning models for non-systematic behavior*, to be submitted to Int. J. Quantum Chem. (published as part of the MSc thesis of C.-Y. Shih).
- M.A. Faiz Afzal, C. Cheng, **J. Hachmann**, *Benchmarking computational protocols for the calculation of polarizability and refractive index values of organic polymers*, to be submitted to J. Chem. Theory Comput.
- A.J. Schultz, **J. Hachmann**, *A multi-junction Scharber model for power conversion efficiency predictions and materials design*, to be submitted to Energy Environ. Sci.
- M. Haghighatlari, C.-Y. Shih, B.A. Moore, Y. Tian, **J. Hachmann**, *ChemML – A machine learning and informatics program suite for the analysis, mining, and modeling of data in the chemical and materials sciences*, to be submitted to J. Chem. Theory Comput.
- W.S. Evangelista, M.A. Faiz Afzal, **J. Hachmann**, *ChemHTPS – A general purpose computational chemistry high-throughput screening platform*, to be submitted to J. Chem. Theory Comput.
- B.A. Moore, A.J. Schultz, **J. Hachmann**, *A numerical survey of the Scharber model for the power conversion efficiencies of organic photovoltaic materials*, to be submitted to Sol. Energy Mater. Sol. Cells.

PUBLICATIONS IN PREPARATION (CONTINUED)

- **J. Hachmann**, K. Rajan, Eds., *Machine Learning and Data-Driven Research in Chemistry: Concepts, Techniques, and Applications*, Wiley, Chichester.

THESES

5. S. Prasad Ganesh, **J. Hachmann**, *How do the geometry differences of isomers affect the polarizability of organic polymers?,* BSc Honors thesis, University at Buffalo – SUNY (**2017**).
4. Y. Tian, **J. Hachmann**, *Inheritance of molecular orbital energies from monomer building blocks to larger copolymers in organic semiconductors*, MSc thesis, University at Buffalo – SUNY (**2016**).
3. C.-Y. Shih, **J. Hachmann**, *Systematic trends in results from different density functional theory models*, MSc thesis, University at Buffalo – SUNY (**2015**).
2. **J. Hachmann**, G.K.-L. Chan, *Ab initio density matrix renormalization group methodology and computational transition metal chemistry*, PhD thesis, Cornell University (**2010**).
1. **J. Hachmann**, N.C. Handy, *Nodal hypersurfaces and sign domains in many-electron wavefunctions*, DiplChem thesis, University of Jena (**2004**).

INVITED TALKS

29. *TBD*, Seminar for the Center for Nonlinear Studies at Los Alamos National Laboratory, Los Alamos (NM), Sep **2017**.
28. *How to Make Data Science Work for Chemistry?*, Chemical Sciences Roundtable of the National Academy of Sciences, Panel on Data Science in Chemistry and Chemical Engineering, Washington (DC), Jul **2017**.
27. *Rational materials design via machine learning*, 253rd ACS National Meeting, CINF Division Symposium on Materials Informatics and Computational Modeling, San Francisco (CA), Apr **2017**.
26. *A data-driven in silico research paradigm for the rational design of catalyst systems*, 253rd ACS National Meeting, CATL Division Symposium on Designed Catalysis: Materials Genome Approach to Heterogeneous Processes, San Francisco (CA), Apr **2017**.
25. *A software ecosystem for data-driven design of chemical systems and the exploration of chemical space*, Workshop on Synergies between Machine Learning and Physical Models, Institute for Pure and Applied Mathematics, Los Angeles (CA), Dec **2016**.
24. *A software ecosystem for data-driven design of chemical systems and the exploration of chemical space*, Theory and Applications of Computational Chemistry 2016, Seattle (WA), Aug **2016**.
23. *A software ecosystem for data-driven design of chemical systems and the exploration of chemical space*, 252nd ACS National Meeting, COMP Division Symposium on Emerging Technologies in Computational Chemistry, Philadelphia (PA), Aug **2016**.
22. *Computational and data-driven discovery of novel high refractive index polymers*, 251st ACS National Meeting, PMSE Division Symposium on Computation and Cheminformatics in Polymers Research, San Diego (CA), Mar **2016**.
21. *Panel Discussion: The Materials Genome and Materials Informatics*, 251st ACS National Meeting, Symposium on Computational Material Science: Theory meets Experiment, San Diego (CA), Mar **2016**.
20. *Data-driven research and a rational design paradigm in the chemical and materials disciplines*, 251st ACS National Meeting, Symposium on Computational Material Science: Theory meets Experiment, San Diego (CA), Mar **2016**.
19. *ChemML – a machine learning and informatics toolbox for the chemical and materials sciences*, Pacifichem 2015, Session on Data Mining and Machine Learning Meets Experiment and First-Principles Simulation for Materials Discovery, Honolulu (HI), Dec **2015**.
18. *Rational materials design via machine learning*, Department Seminar, Department of Physics, University of Vermont, Burlington (VT), Oct **2015**.
17. *Workshop on data mining, machine learning, and materials informatics*, Foundations of Molecular Modeling and Simulation 2015 – Molecular Modeling and the Materials Genome, Mt. Hood (OR), Jul **2015**.
16. *Computing quantum chemical results without doing quantum chemistry: A machine learning shortcut*, 47th Midwest Theoretical Chemistry Conference, Ann Arbor (MI), Jun **2015**.
15. *Molecular properties from big data*, Workshop on Machine Learning for Many-Particle Systems, Institute for Pure and Applied Mathematics, Los Angeles (CA), Feb **2015**.
14. *Molecular properties of organic semiconductors from big data*, MRS Fall Meeting, Symposium on Fundamentals of Organic Semiconductors: Synthesis, Morphology, Devices, and Theory, Boston (MA), Dec **2014**.
13. *Molecular properties from big data*, 248th ACS National Meeting, COMP Division Symposium on Quantum Chemical Calculation of Molecular Properties: A Tribute to Professor Nicholas C. Handy, San Francisco (CA), Aug **2014**.

INVITED TALKS (CONTINUED)

12. *The Harvard Clean Energy Project – a virtual high-throughput search framework for new organic solar cell materials*, 248th ACS National Meeting, ENFL Division Symposium on Applications of Theoretical Chemistry for Energy and Fuel Production, San Francisco (CA), Aug **2014**.
11. *High-throughput quantum chemistry and Big Data techniques for the rational design of organic semiconductors*, Conference on Electronics Materials and Applications 2014, Symposium on Computational Design of Electronic Materials, Orlando (FL), Jan **2014**.
10. *From high-throughput quantum chemistry to the rational design of organic semiconductors – a big data and materials informatics approach*, Department Seminar, Department of Chemistry and Applied Biosciences, Swiss Federal Institute of Technology (ETH) Zürich, Zürich (Switzerland), Oct **2013**.
9. *From high-throughput quantum chemistry to the rational design of organic semiconductors – a big data and materials informatics approach*, CECAM Workshop on Structure-Property Relationships of Molecular Precursors to Organic Electronics, Lausanne (Switzerland), Oct **2013**.
8. *The Harvard Clean Energy Project: High-throughput screening and design of organic photovoltaic materials via automated, first-principles quantum chemistry on the IBM World Community Grid*, 246th ACS National Meeting, PHYS Division Symposium on Physical Chemistry of Solar Energy Conversion, Indianapolis (IN), Sep **2013**.
7. *High-throughput and big data techniques in computational materials science*, 246th ACS National Meeting, COMP Division Symposium on Chemical Mechanisms in Advanced Materials, Indianapolis (IN), Sep **2013**.
6. *Rational design of semiconductors for organic photovoltaics via high-throughput quantum chemistry and materials informatics*, Department Seminar, School of Chemistry, University of Edinburgh, Edinburgh (Scotland), May **2013**.
5. *Rationales Design von Halbleitern für organische Solarzellen durch high-throughput Quantenchemie und Materialinformatik*, Theoretical Chemistry Colloquium, Institute of Physical and Theoretical Chemistry, Braunschweig University of Technology, Braunschweig (Germany), May **2013**.
4. *The Harvard Clean Energy Project: Computational high-throughput screening of OPV materials on the IBM World Community Grid*, Department Seminar, Department of Chemical and Biological Engineering, University at Buffalo, SUNY, Buffalo (NY), Mar **2013**.
3. *The Harvard Clean Energy Project: An automated, high-throughput, first-principles screening of organic photovoltaics on the World Community Grid*, Séminaire du RQMP Versant Nord, Département de physique, Université de Montréal, Montréal (Canada), Mar **2012**.
2. *The Clean Energy Project: Large scale computational search for new organic photovoltaics on the World Community Grid*, Complex Interactions & Mechanisms in Organic Photovoltaics Workshop, Brisbane (Australia), Jul **2010**.
1. *The Harvard Clean Energy Project: A large scale computational search for new organic photovoltaics*, 3rd Puerto Rico NSF EPSCoR/RII IFN Annual Meeting, Rio Grande (PR), May **2010**.

PROFESSIONAL AFFILIATIONS

- Engineers Without Borders USA (EWB-USA) since 2016
- American Ceramic Society (ACerS) 2014
- American Institute of Chemical Engineers (AIChE) since 2013
- Materials Research Society (MRS) since 2012
- Chemical Institute of Canada (CIC) 2009
- World Association of Theoretical and Computational Chemists (WATOC) since 2008
- Psi-k Network since 2008
- Deutsche Physikalische Gesellschaft (DPG) (German Physical Society) since 2006
- American Physical Society (APS) since 2006
- American Chemical Society (ACS) since 2005
- Arbeitsgemeinschaft Theoretische Chemie (AGTC) (Association of German Theoretical Chemists) since 2001
- Deutsche Bunsengesellschaft für Physikalische Chemie (DBG) (German Society for Physical Chemistry) since 2001
- Gesellschaft Deutscher Chemiker (GDCh) (Society of German Chemists) since 2000

PROFESSIONAL SERVICE

SERVICE AS EDITOR

- **Editorial Board Member** for *Scientific Reports* since 2014
- **Editorial Board Member** for *Computational Chemistry Highlights* since 2014
- **Review Editorial Board Member** for *Frontiers in Theoretical and Computational Chemistry* since 2013

PROFESSIONAL SERVICE (CONTINUED)

- **Guest Editor** for *Molecular Systems Design and Engineering* 2017

SERVICE AS REVIEWER AND REFEREE

- **Reviewer (Journals)** for *Accounts of Chemical Research*; *Advanced Energy Materials*; *Australian Journal of Chemistry*; *Chemical Science; Chemistry of Materials*; *ChemPhysChem*; *Computational and Theoretical Chemistry*; *Energy & Environmental Science*; *Frontiers in Theoretical and Computational Chemistry*; *Inorganic Chemistry*; *International Journal of Quantum Chemistry*; *The Journal of Chemical Physics*; *Journal of Chemometrics; Journal of Computational Electronics; Journal of Molecular Modeling; The Journal of Organic Chemistry*; *Journal of Organometallic Chemistry*; *The Journal of Physical Chemistry*; *Journal of the Chilean Chemical Society*; *Macromolecules*; *Materials Discovery*; *Nature Nanotechnology*; *Physical Chemistry Chemical Physics*; *Research on Chemical Intermediates*; *Soft Matter*; *Synthetic Metals*
- **Reviewer (Proposals)** for US National Science Foundation (NSF); US Department of Energy (DOE); American Chemical Society Petroleum Research Fund (ACS PRF); Swiss National Science Foundation (SNSF); Netherlands Organisation for Scientific Research (NWO); Research Foundation Flanders (FWO); Centre Européen de Calcul Atomique et Moléculaire (CECAM); Swiss National Supercomputing Centre (CSCS)
- **Reviewer (Theses)** for University at Buffalo (multiple PhD, MSc in Chemical Engineering, Chemistry); Université de Montréal (PhD in Physics)
- **Jury Member** for the Annual UB CBE Graduate Research Symposium; Annual UB CSTEP Summer Research Poster Symposium; UB Society of Women Engineers Competition; Annual ISEP Science Summit; Annual WNY Regional Science and Engineering Fair; Midwest Theoretical Chemistry Conference; ACS National Meeting PHYS Division

SERVICE AS PROFESSIONAL ADVISOR

- **Advisor** for Mendeley since 2014

SERVICE AS EVENT ORGANIZER

- **Co-Organizer/Co-Chair** of the NSF Division of Chemistry Workshop 2017
  CHE Workshop: Framing the Role of Big Data and Modern Data Science in Chemistry
- **Co-Organizer/Chair** of the PHYS Symposium *Accelerating Discovery: Citizen Science, Big Data, and Machine Learning for Physical Chemistry* at the Fall ACS National Meeting 2016
- **Co-Organizer/Chair** of the CoMSEF/CAST Session *Data-Driven Screening of Chemical and Materials Space* at the AIChE Annual Meeting 2016
- **Co-Organizer/(Co-)Chair** of the CoMSEF Session *Data Mining and Machine Learning in the Molecular Sciences* at the AIChE Annual Meeting since 2015
- **Initiator/Organizer/Chair** of the Annual UB Symposium on *Job and Career Perspectives for Students in the Computational Sciences* since 2015
- **Co-Organizer** of the Annual UB CDSE Days since 2015
- **Co-Organizer** of the Annual UB CBE Graduate Research Symposium since 2014
- **Co-Organizer** of the UB CBE Department Seminar Series since 2014
- **Co-Organizer** of the Greater Boston Area Theoretical Chemistry Lecture Series 2010 – 2014

SERVICE AS COMMUNITY SOFTWARE DEVELOPER

- **Lead-Developer/-Scientist** of the *ChemHTPS*, *ChemBDDB*, and *ChemML* software ecosystem since 2014
- **Developer** for the Q-Chem program package since 2010
- **Lead-Developer/-Scientist** of the Harvard Clean Energy Project Database (CEPDB) 2009 – 2014

SERVICE ON DEPARTMENT COMMITTEES

- **Lead Faculty** of the Student Recruiting and Outreach Committee of the UB CBE Department since 2017
- **Member** of the Graduate Committee of the UB CBE Department; since 2015
  Lead Faculty for student recruiting and McNair Scholars outreach 2015 – 2017
- **Member** of the Curriculum Committee of the UB CDSE Graduate Program since 2015

PROFESSIONAL SERVICE (CONTINUED)

- **Member** of the Faculty Advisory Committee of the UB Center for Computational Research — since 2015
- **Member** of the IT Committee of the UB CBE Department — since 2014
- **Member** of the UB STEM Mentored Undergraduate Research Initiative (SMURI) — 2014

SERVICE ON FACULTY SEARCH COMMITTEES

- **Faculty Search Committee Member** for the UB Department of Mechanical and Aerospace Engineering — 2015
- **Faculty Search Committee Member** for the UB Department of Chemistry — 2014

SERVICE AS FACULTY ADVISOR ON STUDENT INITIATIVES

- **Founding Faculty Advisor** for the UB Student Chapter of Engineers Without Borders (EWB-UB) — since 2016
- **Founding Faculty Advisor** for the UB Graduate Student Association Computational Science Club (CSC) — since 2015

SERVICE IN OUTREACH AND MENTORING

- **Research Mentor** for the Louis Stokes Alliances for Minority Participation (LSAMP) Program — 2017
- **Research Mentor** for the NSF Research Experiences for Undergraduates (REU) Program — 2006, 2008, 2010, 2011

TEACHING EXPERIENCE

- **Instructor, University at Buffalo – SUNY**, Department of Chemical and Biological Engineering
  - *Transport Processes I – Fluid Mechanics* (CE 317, undergraduate) — Fall 2017
    Evaluation: Course: TBD/5, Instructor: TBD/5; Enrollment: 90; Response-Rate: TBD
  - *Computer-Aided Research in the Chemical and Materials Sciences* (CE 451/551, graduate) — Spring 2017
    Evaluation: Course: 3.8/5, Instructor: 4.3/5; Enrollment: 41; Response-Rate: 66%
  - *Transport Processes I – Fluid Mechanics* (CE 317, undergraduate) — Fall 2016
    Evaluation: Course: 4.5/5, Instructor: 4.8/5; Enrollment: 85; Response-Rate: 94%
  - *Special Topics: Computer-Aided Research in the Chemical Sciences* (CE 400/500, graduate) — Spring 2016
    Evaluation: Course: 4.3/5, Instructor: 4.5/5; Enrollment: 39; Response-Rate: 72%
  - *Transport Processes I – Fluid Mechanics* (CE 317, undergraduate) — Fall 2015
    Evaluation: Course: 4.4/5, Instructor: 4.5/5; Enrollment: 85; Response-Rate: 80%
  - *Special Topics: Computer-Aided Research in the Chemical Sciences* (CE 400/500, graduate) — Spring 2015
    Evaluation: Course: 4.2/5, Instructor: 4.5/5; Enrollment: 39; Response-Rate: 72%
  - *Transport Processes I – Fluid Mechanics* (CE 317, undergraduate) — Fall 2014
    Evaluation: Course: 4.5/5, Instructor: 4.6/5; Enrollment: 72; Response-Rate: 76%

- **Guest Instructor, University at Buffalo – SUNY**, Department of Chemical and Biological Engineering
  - *Engineering Impact On Society*, Dr. W.G. Wild, Jr. (EAS 202, undergraduate) — Spring 2017
  - *Engineering Impact On Society*, Dr. W.G. Wild, Jr. (EAS 202, undergraduate) — Spring 2016
  - *Special Topics: Materials Characterization and Properties*, Prof. H. Lin (CE 500, graduate) — Fall 2015
  - *Chemical Engineering Analysis I*, Prof. M. Dupuis (CE 531, graduate) — Fall 2015
  - *Engineering Impact On Society*, Dr. W.G. Wild, Jr. (EAS 202, undergraduate) — Spring 2015
  - *Chemical Engineering Analysis I*, Prof. J.M. Nitsche (CE 531, graduate) — Spring 2015
  - *Special Topics: Materials Characterization and Properties*, Prof. H. Lin (CE 500, graduate) — Fall 2014
  - *Chemical Engineering Analysis I*, Prof. J.M. Nitsche (CE 531, graduate) — Fall 2014
  - *Engineering Impact On Society*, Dr. W.G. Wild, Jr. (EAS 202, undergraduate) — Spring 2014
  - *Chemical Engineering Analysis I*, Prof. J.M. Nitsche (CE 531, graduate) — Spring 2014

- **Workshop Instructor**
  - APS GSOFT Short Course on *Machine Learning and Data Science in Soft Matter*, Los Angeles (CA)
    Machine Learning with Python — Mar 2018
  - FOMMS 2015 – Molecular Modeling and the Materials Genome, Mt. Hood (OR)
    Data Mining, Machine Learning, and Materials Informatics — Jul 2015

TEACHING EXPERIENCE (CONTINUED)

Harvard University, Department of Chemistry and Chemical Biology
Computational Visualization and Modeling Tools for Real-Life Chemical Research Jan 2012

- **Teaching Assistant, Cornell University**, Department of Chemistry and Chemical Biology
  Statistical Mechanics, Prof. B. Widom (CHEM 796, graduate) Spring 2007
  Honors Physical Chemistry I, Prof. J.H. Freed (CHEM 389, undergraduate) Fall 2005

STUDENT MENTORING (AS PRIMARY ADVISOR AT THE UNIVERSITY AT BUFFALO – SUNY)

- Chi Hin Chan (BSc student) since 2017
- Malcolm T. Minnolera (BSc student) since 2017
- Andrew J. Derooy (BSc student) since 2017
- Sykhere A. Brown (BSc student) 2017
- Amol Rajendra Mahajan (MSc student) since 2016
- Aditya Sonpal (MSc student) since 2016
- Gaurav Vishwakarma (MSc student) since 2016
- Po-Han Chen (MSc student) since 2016
- Ryan A. Fair (BSc student; now PhD student at University of Pennsylvania) 2016 – 2017
- Noah A. Zydel (BSc student) since 2016
- Shirish Sivaraj (MSc student) since 2016
- Mark A. Pitman (BSc student; now PhD student at University of Virginia) 2016 – 2017
- Christopher Boulden (BSc student) 2015 – 2017
- Vigneshwar Kumaran Sudalayandi Rajeswari (MSc student) since 2015
- Supriya Agrawal (MSc student) since 2015
- Edward H. Donowick II (BSc student) 2015 – 2017
- Dana M. Havas (BSc student; now PhD student at Cornell University) 2015 – 2016
- William S. Evangelista II (MEng student; now Solutions Engineer at Iconics) 2014 – 2016
- Yujie Tian (MSc student, now Analyst at HSBC) 2014 – 2016
- Yudhajit Pal (PhD student) since 2014
- Anna C. Smith (BSc student; now PhD student at Carnegie Mellon University) 2014 – 2015
- Mikhail Pechagin (BSc student; now Freelance Software Developer in Data Analysis) 2014 – 2016
- Mohammad Atif Faiz Afzal (PhD student) since 2014
- Zachary A. Manzer (BSc student; now PhD student at Cornell University) 2013 – 2015
- Jun Pan (MEng student) 2013 – 2015
- Shawn S. Zadeh (MEng student; now Engineer at Fresenius Kabi) 2013 – 2016
- Ching-Yen Shih (MSc student; now Statistical Programmer at H2O Clinical) 2013 – 2015
- Mojtaba Haghighatlari (PhD student) since 2013
- Sai Prasad Ganesh (BSc student; now PhD student at University of Delaware) 2013 – 2017
- Bryan A. Moore (BSc student; now DOE Mickey Leland Energy Fellow at LANL) 2013 – 2015

Summary: 3 PhD students, 12 MSc/MEng students, 15 BSc students

STUDENT MENTORING (OTHER)

- Akshara Goyal (PhD student, Prof. D. Kofke, University at Buffalo – SUNY) since 2016
- Meghana Nallapu (MSc student, Prof. M. Dupuis, University at Buffalo – SUNY) 2016 – 2017
- Navneeth Gokul (PhD student, Prof. D. Kofke, University at Buffalo – SUNY) since 2016
- Yusen Zhou (PhD student, Prof. S. Neelamegham, University at Buffalo – SUNY) since 2016
- Hanguang Zhang (PhD student, Prof. G. Wu, University at Buffalo – SUNY) since 2016
- Tiange Bi (PhD student, Prof. E. Zurek, University at Buffalo – SUNY) since 2016
- Pavan Kumar Behara (PhD student, Prof. M. Dupuis, University at Buffalo – SUNY) since 2015
- Aparajita Dasgupta (MSc student, Prof. S.J. Park, University at Buffalo – SUNY) 2015 – 2016
- Ramachandran Subramanian (PhD student, Prof. D.A. Kofke, University at Buffalo – SUNY) 2015 – 2016
- Thomas J. Duignan (PhD student, Prof. J. Autschbach, University at Buffalo – SUNY) since 2015
- Alexander V. Marchenko (PhD student, Prof. J. Autschbach, University at Buffalo – SUNY) since 2014

STUDENT MENTORING (CONTINUED)

- Adam R. Rall (PhD student, Prof. J.R. Errington, University at Buffalo – SUNY) since 2014
- Martin A. Blood-Forsythe (PhD student, Prof. A. Aspuru-Guzik, Harvard University) 2012 – 2014
- Supriya Shrestha (MSc student, Prof. A. Aspuru-Guzik, Harvard University) 2012 – 2013
- László R. Seress (BSc student, Prof. A. Aspuru-Guzik, Harvard University) 2011 – 2014
- Alexander Shlomo Ramek (BSc student, Prof. A. Aspuru-Guzik, Harvard University) 2011 – 2012
- Leon Xueliang Liu (PhD student, Prof. A. Aspuru-Guzik, Harvard University) 2011 – 2012
- James H. Zhu (REU student, Prof. A. Aspuru-Guzik, Cornell University) 2011
- Anna M. Brockway (REU student, Prof. A. Aspuru-Guzik, Haverford College) 2010
- Lauren A. Kaye (BSc student, Prof. A. Aspuru-Guzik, Harvard University) 2010 – 2011
- Aryeh Gold-Parker (BSc student, Prof. A. Aspuru-Guzik, Harvard University) 2009 – 2012
- Roberto Olivares-Amaya (PhD student, Prof. A. Aspuru-Guzik, Harvard University) 2009 – 2012
- Eduardo Márquez (REU student, Prof. G.K.-L. Chan, University of Puerto Rico, Mayagüez) 2008
- Michael Avilés (REU student, Prof. G.K.-L. Chan, Arcadia University) 2006
- Tony Chu (BSc student, Prof. G.K.-L. Chan, Cornell University) 2004 – 2006

Summary: 13 PhD students, 3 MSc/MEng students, 9 BSc/REU students

STUDENT AWARDS & HONORS

- Scholarship Award for Scientific Excellence of the ACS Division of Chemical Information (Mohammad Atif Faiz Afzal) 2017
- 1st Prize of the Buffalo Student SandBox Competition (Mohammad Atif Faiz Afzal) 2017
- People's Choice Award of the Bright Buffalo Niagara Entrepreneur Expo (Mohammad Atif Faiz Afzal) 2017
- WNY-ACS Distinguished Student Award (Ryan Fair) 2017
- UB CBE Senior Academic Excellence Award (Sai Prasad Ganesh) 2017
- UB Louis Stokes Alliance for Minority Participation Summer Research Internship (Sykhere Brown) 2017
- UB 3MT Competition Finalist (Mohammad Atif Faiz Afzal) 2017
- UB Presidential Fellowship (Ryan Fair, declined) 2017
- UB Presidential Fellowship (Sai Prasad Ganesh, declined) 2017
- UB SEAS Senior Scholars Research Scholarship (Ryan Fair) 2017
- UB SEAS Senior Scholars Research Scholarship (Sai Prasad Ganesh) 2017
- Winner of the UB Hackathon (Mohammad Atif Faiz Afzal, Edward H. Donowick II) 2016
- IPAM Travel Grant (Mohammad Atif Faiz Afzal) 2016
- UB SEAS Dean's List (Ryan Fair) 2016 – 2017
- Graduate Student Grant of the Mark Diamond Research Fund (Mohammad Atif Faiz Afzal) 2016
- IPAM Long Program Housing and Travel Grant (Mojtaba Haghighatlari) 2016
- UB CBE Best Poster Award (Mojtaba Haghighatlari) 2016
- APS Distinguished Student Travel Award (Mohammad Atif Faiz Afzal) 2016
- Outstanding Student Poster Award of the ACS Physical Chemistry Division (Mojtaba Haghighatlari) 2016
- Scholarship Award for Scientific Excellence of the ACS Division of Chemical Information (Mojtaba Haghighatlari) 2016
- 1Sα Poster Prize of the Midwest Theoretical Chemistry Conference (Mohammad Atif Faiz Afzal) 2016
- 2016 UB CBE Graduate Student Seminar Speaker (Mohammad Atif Faiz Afzal) 2016
- UB SEAS Senior Academic Excellence Award of the UB CBE Department (Dana M. Havas) 2016
- Honorable Mention for the NSF Graduate Research Fellowship (Dana M. Havas) 2016
- Professor Emeritus Howard Strauss Memorial Scholarship Award of the UB Engineering Alumni Association (Mohammad Atif Faiz Afzal) 2016
- Honorable Mention for the Ovshinsky Student Travel Award of the APS Division of Materials Physics (Mohammad Atif Faiz Afzal) 2016
- UB Honors College Advanced Honors Scholar (Sai Prasad Ganesh) 2015
- TSTC Travel Grant (Mohammad Atif Faiz Afzal) 2015
- UB SEAS Dean's List (Sai Prasad Ganesh) 2014 – 2016
- UB SMURI Summer Research Award (Bryan A. Moore) 2014

PENDING GRANTS & FUNDING

- NSF CISE OAC Early Career Development Program, $562k: 2018 – 2023
  CAREER: Building an Advanced Cyberinfrastructure for the Data-Driven Design of Chemical Systems and the Exploration of Chemical Space
- NSF IIS Big Data Spokes Program (with V. Govindaraju, K. Rajan, G. Hutchison, *et al.*), $1M: 2018 – 2021
  Spokes: MEDIUM: NORTHEAST: Advancing a Data-Driven Discovery and Rational Design Paradigm in Chemistry
- NSF Major Research Instrumentation Program (with T. Furlani, *et al.*), $1.4M: 2017 – 2018
  MRI: Acquisition of High-Performance Computing Infrastructure to Support Computational and Data-Enabled Science and Engineering