CURRICULUM VITAE

Michael John Schnieders

June 2022

I. EDUCATIONAL AND PROFESSIONAL HISTORY

A. List of institutions attended (earliest to most recent)

1999	BSE (Biomedical Engineering) - The University of Iowa, Iowa City, Iowa, United States High Distinction
2007	DSc (Biomedical Engineering) - Washington University in St. Louis, St. Louis, Missouri, United States

Post Graduate

2007 - 2010	Postdoctoral Fellow (Chemistry) - Stanford University, Stanford, California, United States Mentor: Vijay S Pande
2011 - 2012	Postdoctoral Fellow (Biomedical Engineering) - The University of Texas, Austin, Texas, United States Mentor: Pengyu Ren

B. Employment History

2012 - 2018	Assistant Professor, Biochemistry The University of Iowa, Iowa City, Iowa, United States
2012 - 2018	Assistant Professor, Biomedical Engineering The University of Iowa, Iowa City, Iowa, United States
2019 - 2020	Harrington Fellow, Biomedical Engineering The University of Texas at Austin, Austin, Texas, United States
2018 - Present	Associate Professor, Biochemistry and Molecular Biology The University of Iowa, Iowa City, Iowa, United States
2018 - Present	Associate Professor, Biomedical Engineering The University of Iowa, Iowa City, Iowa, United States

C. Honors, Awards, Recognitions, Outstanding Achievements

1995 - 1996	Stebler Scholarship - The University of Iowa
1996 - 1997	Paul D. Scholz Memorial Scholarship - The University of Iowa
1997 - 1998	National Barry Goldwater Excellence in Education Scholarship - The University of Iowa
1998 - 1999	Rhodes Dunlap Scholarship - The University of Iowa
2001 - 2004	Grace Norman Graduate Fellowship - Washington University in St. Louis
2004 - 2006	NIH Biophysics Training Grant Fellowship - Washington University in St. Louis
2010	Best Poster Award - Electron Density and Chemical Bonding Gordon Research Conf, Stanford University

2012 - 2013	Burroughs Wellcome Fund Travel Award - The University of Texas at Austin
2018	Honors' Scholar Advocate Award - The University of Iowa
2019 - 2020	Donald D. Harrington Faculty Fellow - University of Texas at Austin
2018 - 2023	CAREER Award - National Science Foundation
2022	Iowa Mid-Career Faculty Scholar Award - The University of Iowa

II. TEACHING

A. Teaching assignments

Classroom, Seminar, Teaching Laboratory

Spring 2013	ENGR:1300 Engineering Problem Solving II (3 s.h), Primary Instructor (100%) *45 Lectures for 56 Students*
Fall 2013	ENGR:1300 Engineering Problem Solving II (3 s.h), Primary Instructor (100%) *45 Lectures for 65 Students*
Spring 2014	BME:2200 Systems, Instrumentation & Data Acquisition (4 s.h.), Course Supervisor (50%) *24 lectures and 8 labs (3 hrs/each) for 64 students.*
Fall 2014	BME:2200 Systems, Instrumentation & Data Acquisition (4 s.h.), Course Supervisor (50%) *24 lectures and 8 labs (3 hrs/each) for 41 students.*
Spring 2015	BME:2210 Bioimaging and Bioinformatics (4 s.h.), Course Supervisor (50%) *23 lectures for 72 students.*
Fall 2015	BME:2210 Bioimaging and Bioinformatics (4 s.h.), Course Supervisor (50%) *23 lectures for 40 students.*
Fall 2015	BME:4310 Computational Biochemistry (3 s.h.), Course Supervisor (100%) *30 lectures (75 min./each) for 19 students.*
Fall 2016	BME:2210 Bioimaging and Bioinformatics (4 s.h.), Course Supervisor (50%) *23 lectures for 53 students.*

Fall 2016	BME:4310 Computational Biochemistry (3 s.h.), Course Supervisor (100%) *30 lectures (75 min./each) for 21 students.*
Fall 2017	BME:2210 Bioimaging and Bioinformatics (4 s.h.), Course Supervisor (50%) *24 lectures for 53 students.*
Fall 2017	BME:4310 Computational Biochemistry (3 s.h.), Course Supervisor (100%) *30 lectures (75 min./each) for 20 students.*
Fall 2018	BME:4310 Computational Biochemistry (3 s.h.), Course Supervisor (100%) *30 lectures (75 min./each) for 12 students.*
Fall 2020	BME:4310 Computational Biochemistry (3 s.h.), Course Supervisor (100%) *30 lectures (75 min./each) for 31 students.*
Spring 2021	BME:2210 Bioimaging and Bioinformatics (4 s.h.), Course Supervisor (50%) *24 lectures and 6 labs for 67 students.*
Fall 2021	BME:2210 Bioimaging and Bioinformatics (4 s.h.), Course Supervisor (50%) *24 lectures and 6 labs for 29 students.*
Spring 2022	BME:2210 Bioimaging and Bioinformatics (4 s.h.), Course Supervisor (50%) *24 lectures and 6 labs for 57 students.*

B. Student Supervision

Graduate Students

2014 - 2015	Jooyeon Park - Biomedical Engineering - BS/MS Fast Track The University of Iowa *Completed Dental School at the U. of Penn.*
2014 - 2016	Armin Avdic - Biomedical Engineering - MS The University of Iowa *Completed Medical School at the Carver College of Medicine.*
2016 - 2017	Mallory Tollefson - Biomedical Engineering - BS/MS Fast Track The University of Iowa *2018 NSF Graduate Fellowship* *Thesis Project: Development of the OtoProtein Database to Support Genetic Testing for Deafness for Clinical Diagnostics*

2014 - 2017 Stephen LuCore - Biomedical Engineering - MS
The University of Iowa

2016 - 2017 Timothy Collingsworth - Biochemistry - MS
The University of Iowa
Next Position: Research assistant with Prof. Adrian Elcock at the U. of Iowa.

2014 - 2019 Jacob Litman - Biochemistry - PhD
The University of Iowa
2014 Presidential Graduate Research Fellowship
2015 CBB Predoctoral Training Program
Thesis Project: Advanced Optimization and Sampling Techniques for Biomolecules Using a Polarizable Force Field
Next Position: Postdoctoral Fellow at UT Austin

2016 - 2019 Hernan Bernabe - Biomedical Engineering - MS
The University of Iowa
2017 CBB Predoctoral Training Program

2017 - Present Mallory Tollefson - Biomedical Engineering - PhD
The University of Iowa
2018 NSF Graduate Research Fellowship
2021 American Association of University Women Graduate Fellowship

2017 - Present Rae Corrigan - Biomedical Engineering - PhD
The University of Iowa
2015 ICRU Scholarship
2016 Goldwater Excellence in Education Scholarship
2018 NSF Graduate Research Fellowship
2021 Internship at Integrated DNA Technologies (IDT) Internship
2022 Ballard and Seashore Dissertation Fellowship

2018 - Present Aaron Nessler - Biomedical Engineering - PhD
The University of Iowa
2018 *Internship at Mitsubishi Tanabe Pharma in Tokyo, Japan*

2019 - Present Andrew Thiel - Biomedical Engineering - PhD
The University of Iowa
2018 Summer Internship at Pfizer, Groton, CT
2020 NSF Graduate Research Fellowship

2020 - Present Rose Gogal - Biomedical Engineering - Ph.D.
The University of Iowa
2020 Graduate College Recruitment Fellowship
2021 CBB Predoctoral Training Program

Medical Students

2016 - 2019 Armin Avdic - Medical School - MD
The University of Iowa
2016 College of Medicine Summer Research Fellowship

2018 - 2021 Soham Ali - Medical School - MD
The University of Iowa
2018 College of Medicine Summer Research Fellowship

Postdoctoral Research Supervision

2019 - 2020	Jacob Litman - Post-Doctoral Fellow - Biomedical Engineering University of Texas at Austin

Thesis Committee

2014 - 2016	Jeevapani Hettige - Chemistry - PhD The University of Iowa
2012 - 2017	Shuxiang Li - Biochemistry - PhD The University of Iowa
2013 - 2017	Young Joo Sun - Biochemistry - PhD The University of Iowa
2014 - 2017	Cheng Zhou - Biomedical Engineering - PhD The University of Iowa
2012 - 2018	Kyle Powers - Biochemistry - PhD The University of Iowa
2013 - 2018	Wesley Lay - Biochemistry - PhD The University of Iowa
2014 - 2018	Aditya Singaraju - Pharmaceutical Sciences and Experimental Therapeutics - PhD The University of Iowa
2014 - 2019	Melissa Gildenberg - Biochemistry - PhD The University of Iowa
2014 - 2020	Will Hacker - Biochemistry - PhD The University of Iowa
2014 – 2021	Robert McDonnell - Biochemistry - PhD The University of Iowa
2015 – 2021	Zaid Assaf - Pharmacology - PhD The University of Iowa
2019 - 2022	Jin-Young Koh - Genetics - PhD The University of Iowa
2019 – 2022	Beth Young - Pharmacology - PhD The University of Iowa
2019 - 2022	Dherya Bahl - Pharmacology - PhD The University of Iowa
2016 - Present	Venkata Sanaboyana - Biochemistry - PhD The University of Iowa
2017 - Present	Zachary Wehrspan - Biochemistry - PhD The University of Iowa
2020 - Present	Emily Landgreen - Chemistry - PhD The University of Iowa
2020 - Present	Hayley Petras - Chemistry - PhD The University of Iowa
2021 - Present	Monique Weaver - Genetics - PhD The University of Iowa

2021 - Present Lucas Pietan – Biomedical Engineering - PhD
The University of Iowa

Undergraduate Students

2013 - 2016 Ian Nessler - Chemical Engineering - BSE
The University of Iowa
2014 Internship at Genentech in San Francisco
2015 ICRU Scholarship
2016 NSF Graduate Fellowship Recipient
Next Position: 2021 Chemical Engineering PhD from U. Michigan

2015 - 2016 Jill Hauer - Biomedical Engineering - BSE
The University of Iowa
2017 NSF Graduate Fellowship Recipient
Next Position: 2021 Genetics PhD from the U. of Iowa

2014 - 2017 Rae Corrigan - Biomedical Engineering - BSE
The University of Iowa
2016 ICRU Scholarship
2016 Goldwater Excellence in Education Scholarship
2018 NSF Graduate Fellowship
Next Position: Iowa BME PhD Student

2016 - 2019 Claire O'Connell - Biomedical Engineering - BSE
The University of Iowa
2018 ICRU Scholarship
Next Position: Goldman Sachs

2017 – 2021 Guowei Qi - Undergraduate Student - Biochemistry - BS
The University of Iowa
2019 Barry Goldwater Scholarship
2021 NSF Graduate Research Fellowship
2021 Churchill Scholarship
Next Position: D.E. Shaw Research

2020 - Present Jack Lynn - Biomedical Engineering - B.S.E.
The University of Iowa
2021 Barry Goldwater Scholarship
Next Position: Genesis10

2020 - Present Kaleb Bierstedt - Biomedical Engineering, Biochemistry - B.S.E.
The University of Iowa
2021 ICRU Scholarship

2021 - Present Mitchell Hermon – Computer Science - B.S.
The University of Iowa
2022 Summer Internship at Amazon, Austin, TX

2021 – Present Risha Shetye – Chemical Engineering - B.S.E.
The University of Iowa
2022 ICRU Scholarship

III. SCHOLARSHIP/PROFESSIONAL PRODUCTIVITY

A. Publications or creative works (earliest to most recent)

Peer-reviewed papers and journal articles

1. Schnieders MJ, Dave SB, Morrow DE, Heiner AD, Pedersen DR, Brown TD. Assessing the accuracy of a prototype drill guide for fibular graft placement in femoral head necrosis, Iowa Orthopaedic Journal. 1997;17:58-63.
2. Anderson DA, Schnieders MJ, Heiner AD, Pederson DR, Brown TD, Brand RA. A surgical guide to accurately place pins or nails within the femoral head, Journal of Musculoskeletal Research. 1999;3:233-237. doi: 10.1142/S0218957799000245.
3. Schnieders MJ, Ponder JW. Polarizable atomic multipole solutes in a generalized Kirkwood continuum, Journal of Chemical Theory and Computation. 2007;3(6):2083-2097. doi: 10.1021/ct7001336.
4. Schnieders MJ, Baker NA, Ren P, Ponder JW. Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum, Journal of Chemical Physics. 2007;126(12):124114. doi: 10.1063/1.2714528.
5. Mathew-Fenn RS, Das R, Fenn TD, Schnieders MJ, Harbury P. Response to comment on "Remeasuring the double helix", Science. 2009 July;325(5940):538. doi: 10.1126/science.1168876.
6. MacCallum JL, Hua L, Schnieders MJ, Pande VS, Jacobson MP, Dill KA. Assessment of the protein-structure refinement category in CASP8, Proteins: Structure, Function, and Bioinformatics. 2009;77(S9):66-80. PMID:19714776. PMCID: PMC2801025. doi: 10.1002/prot.22538.
7. Schnieders MJ, Fenn TD, Pande VS, Brunger AT. Polarizable atomic multipole X-ray refinement: Application to peptide crystals, Acta Crystallographica Section D. 2009;65(9):952-965. doi: 10.1107/S0907444909022707.
8. Jiao D, Zhang JJ, Duke RE, Li GH, Schnieders MJ, Ren P. Trypsin-ligand binding free energies from explicit and implicit solvent simulations with polarizable potential, Journal of Computational Chemistry. 2009;30(11):1701-1711. doi: 10.1002/jcc.21268.
9. Shi Y, Jiao D, Schnieders MJ, Ren P. Trypsin-ligand binding free energy calculation with AMOEBA, Conference proceedings: Annual International Conference of the IEEE Engineering in Medicine and Biology Society. IEEE Engineering in Medicine and Biology Society. Conference. 2009;2009:2328-31. PMID:19965178. PMCID: PMC2819397. doi: 10.1109/IEMBS.2009.5335108.
10. Fenn TD, Schnieders MJ, Brunger AT, Pande VS. Polarizable atomic multipole x-ray refinement: hydration geometry and application to macromolecules, Biophysical Journal. 2010 June;98(12):2984-2992. PMID:20550911. PMCID: PMC2884231. doi: 10.1016/j.bpj.2010.02.057.
11. Fenn TD, Schnieders MJ, Brunger AT. A smooth and differentiable bulk-solvent model for macromolecular diffraction, Acta Crystallographica Section D. 2010;66(9):1024-1031. doi: 10.1107/S0907444910031045.
12. Ponder JW, Wu C, Ren P, Pande VS, Chodera JD, Schnieders MJ, Haque I, Mobley DL, Lambrecht DS, DiStasio RA, Head-Gordon M, Clark GN I, Johnson ME, Head-Gordon T. Current status of the AMOEBA polarizable force field, Journal of Physical Chemistry B. 2010;114(8):2549-2564. doi: 10.1021/jp910674d.

13. Schnieders MJ, Fenn TD, Pande VS. Polarizable atomic multipole X-ray refinement: Particle mesh Ewald electrostatics for macromolecular crystals, Journal of Chemical Theory and Computation. 2011 March 9;7(4):1141-1156. doi: 10.1021/ct100506d.

14. Fenn TD, Schnieders MJ, Mustyakimov M, Wu C, Langan P, Pande VS, Brunger AT. Reintroducing electrostatics into macromolecular crystallographic refinement: application to neutron crystallography and DNA hydration, Structure. 2011 April;19(4):523-533. PMID:21481775. PMCID: PMC3083928. doi: 10.1016/j.str.2011.01.015.

15. MacCallum JL, Pérez A, Schnieders MJ, Hua L, Jacobson MP, Dill KA. Assessment of protein structure refinement in CASP9, Proteins: Structure, Function, and Bioinformatics. 2011 August 30;79(S10):74-90. PMID:22069034. PMCID: PMC3238793. doi: 10.1002/prot.23131.

16. Fenn TD, Schnieders MJ. Polarizable atomic multipole X-ray refinement: weighting schemes for macromolecular diffraction, Acta Crystallographica Section D. 2011 November;67(11):957-965. PMID:22101822. PMCID: 22101822. doi: 10.1107/S0907444911039060.

17. MacCallum JL, Pérez A, Schnieders MJ, Hua L, Jacobson MP, Dill KA. Assessment of protein structure refinement in CASP9, Proteins: Structure, Function, and Bioinformatics. 2011;79(S10):74-90. doi: 10.1002/prot.23131.

18. Schnieders MJ, Fenn TD, Pande VS. Polarizable atomic multipole X-ray refinement: Particle mesh Ewald electrostatics for macromolecular crystals, Journal of Chemical Theory and Computation. 2011;7(4):1141-1156.

19. Fenn TD, Schnieders MJ, Mustyakimov M, Wu C, Langan P, Pande VS, Brunger AT. Reintroducing electrostatics into macromolecular crystallographic refinement: application to neutron crystallography and DNA hydration, Structure. 2011;19(4):523-533.

20. Ren P, Chun J, Thomas DG, Schnieders MJ, Marucho M, Zhang J, Baker NA. Biomolecular electrostatics and solvation: a computational perspective, Quarterly Reviews of Biophysics. 2012 November;45(4):427-491. PMID:23217364. PMCID: PMC3533255. doi: 10.1017/S003358351200011X.

21. Ren P, Chun J, Thomas DG, Schnieders MJ, Marucho M, Zhang J, Baker NA. Biomolecular electrostatics and solvation: a computational perspective, Quarterly Reviews of Biophysics. 2012;45(4):427-491. doi: 10.1017/S003358351200011X.

22. Schnieders MJ, Kaoud TS, Yan C, Dalby KN, Ren P. Computational insights for the discovery of non-ATP competitive inhibitors of MAP kinases, Current Pharmaceutical Design. 2012;18(9):1173-1185. PMID:22316156. PMCID: PMC4016787. doi: 10.2174/138920012799362873.

23. Schnieders MJ, Baltrusaitis J, Shi Y, Chattree G, Zheng L, Yang W, Ren P. The structure, thermodynamics, and solubility of organic crystals from simulation with a polarizable force field, Journal of Chemical Theory and Computation. 2012;8(5):1721-1736. doi: 10.1021/ct300035u.

24. Park J, Nessler I, McClain B, Macikenas D, Baltrusaitis J, Schnieders MJ. Absolute organic crystal thermodynamics: Growth of the asymmetric unit into a crystal via alchemy, Journal of Chemical Theory and Computation. 2014;10(7):2781-2791. doi: 10.1021/ct500180m.

25. Lipparini F, Lagardère L, Stamm B, Cancès E, Schnieders MJ, Ren P, Maday Y, Piquemal J-P. Scalable evaluation of polarization energy and associated forces in polarizable molecular dynamics: I. Toward massively parallel direct space computations, Journal of Chemical Theory and Computation. 2014;10(4):1638-1651. doi: 10.1021/ct401096t.

26. Lipparini F, Lagardère L, Raynaud C, Stamm B, Cancès E, Mennucci B, Schnieders MJ, Ren P, Maday Y, Piquemal J-P. Polarizable molecular dynamics in a polarizable continuum solvent, Journal of Chemical Theory and Computation. 2015 January 26;11(2):623-634. doi: 10.1021/ct500998q.

27. Shi Y, Schnieders MJ, Piquemal J-P, Ren P. Polarizable force fields for biomolecular modeling, Reviews in Computational Chemistry. 2015 May 1;28:51-86. doi: 10.1002/9781118889886.ch2.

28. Lagardère L, Lipparini F, Polack É, Stamm B, Cancès É, Schnieders MJ, Ren P, Maday Y, Piquemal J-P. Scalable evaluation of polarization energy and associated forces in polarizable molecular dynamics: II. Toward massively parallel computations using smooth particle mesh Ewald, Journal of Chemical Theory and Computation. 2015 May 21;11(6):2589-2599. doi: 10.1021/acs.jctc.5b00171.

29. LuCore SD, Litman JM, Powers KT, Gao S, Lynn AM, Tollefson WT A, Fenn TD, Washington MT, Schnieders MJ. Dead-end elimination with a polarizable force field repacks PCNA structures, Biophysical Journal. 2015 August 18;109(4):816-826. doi: 10.1016/j.bpj.2015.06.062.

30. Booth KT, Azaiez H, Kahrizi K, Simpson AC, Tollefson WTA, Sloan CM, Meyer NC, Babanejad M, Ardalani F, Arzhangi S, Schnieders MJ, Najmabadi H, Smith RJH. PDZD7 and hearing loss: More than just a modifier, American Journal of Medical Genetics Part A. 2015 September 29. doi: 10.1002/ajmg.a.37274.

31. Bell DR, Qi R, Jing Z, Xiang JY, Mejias C, Schnieders MJ, Ponder JW, Ren P. Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field, Physical Chemistry Chemical Physics. 2016;18(44):30261-30269. doi: 10.1039/C6CP02509A.

32. Bu F, Borsa NG, Jones MB, Takanami E, Nishimura C, Hauer JJ, Azaiez H, Black-Ziegelbein EA, Meyer NC, Kolbe DL, Li Y, Frees K, Schnieders MJ, Thomas C, Nester C, Smith RJH. High-Throughput Genetic Testing for Thrombotic Microangiopathies and C3 Glomerulopathies, Journal of the American Society of Nephrology. 2016;27(4):1245-1253. doi: 10.1681/asn.2015040385.

33. DeLuca AP, Whitmore SS, Barnes J, Sharma TP, Westfall TA, Scott CA, Weed MC, Wiley JS, Wiley LA, Johnston RM, Schnieders MJ, Lentz SR, Tucker BA, Mullins RF, Scheetz TE, Stone EM, Slusarski DC. Hypomorphic mutations in TRNT1 cause retinitis pigmentosa with erythrocytic microcytosis, Human Molecular Genetics. 2016;25(1):44-56. doi: 10.1093/hmg/ddv446.

34. Nessler IJ, Litman JM, Schnieders MJ. Toward polarizable AMOEBA thermodynamics at fixed charge efficiency using a dual force field approach: application to organic crystals, Physical Chemistry Chemical Physics. 2016;18(44):30313-30322. doi: 10.1039/C6CP02595A.

35. Simpson A, Avdic A, Roos BR, DeLuca A, Miller K, Schnieders MJ, Scheetz TE, Alward WLM, Fingert JH. LADD syndrome with glaucoma is caused by a novel gene, Molecular Vision. 2017 March 30;23:179-184.

36. Lansdon LA, Bernabe HV, Nidey N, Standley J, Schnieders MJ, Murray JC. The Use of Variant Maps to Explore Domain-Specific Mutations of FGFR1, Journal of Dental Research. 2017 October 1;96(11):1339-1345. doi: 10.1177/0022034517726496.

37. Lagardère L, Jolly LH, Lipparini F, Aviat F, Stamm B, Jing ZF, Harger M, Torabifard H, Cisneros GA, Schnieders MJ, Gresh N, Maday Y, Ren PY, Ponder JW, Piquemal JP. Tinker-HP: A massively parallel molecular dynamics package for multiscale simulations

of large complex systems with advanced point dipole polarizable force fields, Chemical Science. 2018 January 1;9(4):956-972. doi: 10.1039/c7sc04531j.

38. Schnieders MJ, Goar W, Griess M, Roos BR, Scheetz TE, Stone EM, Fingert JH. A novel mutation (LEU396ARG) in OPA1 is associated with a severe phenotype in a large dominant optic atrophy pedigree, Eye. 2018 April 1;32(4):843-845. PMID:29350691. PMCID: PMC5898874. doi: 10.1038/eye.2017.303.

39. Azaiez H, Booth KT, Ephraim SS, Crone B, Black-Ziegelbein EA, Marini RJ, Shearer AE, Sloan-Heggen CM, Kolbe D, Casavant T, Schnieders MJ, Nishimura C, Braun T, Smith RJ. Genomic Landscape and Mutational Signatures of Deafness-Associated Genes., American Journal of Human Genetics. 2018 October 4;103(4):484-497. PMID:30245029. PMCID: PMC6174355. doi: 10.1016/j.ajhg.2018.08.006.

40. Rackers JA, Wang Z, Lu C, Laury ML, Lagardère L, Schnieders MJ, Piquemal JP, Ren P, Ponder JW. Tinker 8: Software Tools for Molecular Design., Journal of Chemical Theory and Computation. 2018 October 9;14(10):5273-5289. PMID:30176213. PMCID: PMC6335969. doi: 10.1021/acs.jctc.8b00529.

41. Tollefson MR, Litman JM, Qi G, O'Connell CE, Wipfler MJ, Marini RJ, Bernabe HV, Tollefson WTA, Braun TA, Casavant TL, Smith RJH, Schnieders MJ. Structural Insights into Hearing Loss Genetics from Polarizable Protein Repacking., Biophysical journal. 2019 August 6;117(3):602-612. PMID:31327459. PMCID: PMC6697528. doi: 10.1016/j.bpj.2019.06.030.

42. Litman J, Thiel AC, Schnieders MJ. Scalable Indirect Free Energy Method Applied to Divalent Cation-Metalloprotein Binding., Journal of Chemical Theory and Computation. 2019 August 13;15(8):4602-4614. PMID:31268700. doi: 10.1021/acs.jctc.9b00147.

43. Boese EA, Tollefson MR, Schnieders MJ, Darbro BW, Alward WLM, Fingert JH. Novel Intragenic *PAX6* Deletion in a Pedigree with Aniridia, Morbid Obesity, and Diabetes., Current Eye Research. 2020 January 1;45(1):91-96. PMID:31361967. doi: 10.1080/02713683.2019.1649704.

44. Bi J, Thiel KW, Litman JM, Zhang Y, Devor EJ, Newtson AM, Schnieders MJ, Gonzalez Bosquet J, Leslie KK. Characterization of a TP53 Somatic Variant of Unknown Function From an Ovarian Cancer Patient Using Organoid Culture and Computational Modeling., Clinical obstetrics and gynecology. 2020 March 1;63(1):109-119. PMID:31876640. doi: 10.1097/GRF.0000000000000516.

45. Hagedorn J, Avdic A, Schnieders MJ, Roos BR, Kwon YH, Drack AV, Boese EA, Fingert JH. Nanophthalmos patient with a THR518MET mutation in MYRF, a case report., BMC ophthalmology. 2020 October 1;20(1):388. PMID:33004036. PMCID: PMC7528587. doi: 10.1186/s12886-020-01659-8.

46. Corrigan RA, Qi G, Thiel AC, Lynn JR, Walker BD, Casavant TL, Lagardere L, Piquemal J-P, Ponder JW, Ren P, Schnieders MJ. Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field, Journal of Chemical Theory and Computation. 2021;17(4):2323-2341. doi: 10.1021/acs.jctc.0c01286.

47. Qi G, Tollefson MR, Gogal RA, Smith RJH, AlQuraishi M, Schnieders MJ, Protein Structure Prediction Using a Maximum Likelihood Formulation of a Recurrent Geometric Network. bioRxiv 2021, doi: 0.1101/2021.09.03.45887

48. Hinz BE, Walker SG, Xiong A, Gogal RA, Schnieders MJ, Wallrath LL, In Silico and In Vivo Analysis of Amino Acid Substitutions That Cause Laminopathies. International Journal of Molecular Sciences 2021, 22 (20), 11226. doi: 10.3390/ijms222011226.

49. Awotoye W, Mossey P, Hetmanski J, Gowans LJJ, Eshete M, Adeyemo W, Alade A, Zeng E, Adamson O, Naicker T, Anand D, Adeleke C, Busch T, Li M, Petrin A,

Aregbesola B, Braimah R, Oginni F, Oladele A, Oladayo A, Kayali S, Olotu J, Hassan M, Pape J, Donkor P, Arthur FKN, Obiri-Yeboah S, Sabbah D, Agbenorku P, Plange-Rhule G, Oti AA, Gogal R, Beaty T, Taub M, Marazita M, Schnieders M, Lachke S, Adeyemo A, Murray J, Butali A, Whole-genome Sequencing Reveals De-novo Mutations Associated with Nonsyndromic Cleft Lip/Palate. 2022 (*under review*).

B. Areas of Research Interest

Chemical Theory for the Protein Crystal Folding Problem.

Computational prediction of the structure, space group, unit cell parameters and stability of protein crystals remains an unsolved problem, despite the importance of polymer crystals to life science research and industrial applications such as formulation of peptide therapeutics. We have demonstrated novel approaches to discover peptide polymorphs using thermodynamically driven search algorithms.

Next Generation Theory and Tools for Biomolecular Simulation.

Many of the most widely used computational biochemistry software programs have been written over many decades in languages such as C and FORTRAN. However, emerging high-level languages that execute on the Java Virtual Machine, such as Java, Groovy, Scala and Kotlin, couple with low-level GPU languages, such as CUDA and OpenCL, represent a new paradigm in software development. Our lab is exploring this paradigm our software program Force Field X, which couples high-level JVM code accelerated by the OpenMM GPU API.

Physics-Based Simulations of the Genetics of Hearing Loss.

Hearing loss is the most common sensory deficit and is contributed to by genetic variations identified in more than 100 genes. These variations are being catalogued at the University of Iowa by a collaboration led by Dr. Richard Smith and disseminated to the community using the Deafness Variation Database (DVD at http://deafnessvariationdatabase.org). Currently most variations in the DVD (700,000 out of more than 800,000) are of unknown significance. To address this, we're developing atomic resolution physics-based models the implicated proteins to understand their molecular phenotypes.

Physics-Based Simulations of the Genetics of Renal Disease.

Renal disease (i.e. C3G) can arise from mis-regulation of the complement system. We are using physics-based simulations to 1) understand the molecular phenotypes of complement proteins and their associated missense variations 2) to improve the potency of established peptide based inhibitors of C3 (e.g. compstatin).

C. Grants

Grant

Funded

Optimizing Genetic Testing for Deafness for Clinical Diagnostics
National Institutes of Health
R01DC012049
December 5, 2016 - November 30, 2026
$2,570,030
Percent effort: 10
Smith, Richard J. (Principal Investigator), Schnieders, Michael J (Multi-PI), Braun, Terry (Multi-PI), Casavant, Thomas (Multi-PI)

CAREER: Chemical Theory for the Protein Crystal Folding Problem
National Science Foundation
CHE-1751688
April 1, 2018 - March 31, 2024
$705,521
Percent effort: 8.33
Schnieders, Michael J. (Principal Investigator)

Completed

Chemistry of Mitochondrial Protein Acetylation: Evolution of Substrate Reactivity as a Regulatory Mechanism
National Science Foundation
CHE-1404147
July 1, 2014 - June 20, 2017
$504,000
Percent effort: 8.3
Brenner, Charles (Principal Investigator), Schnieders, Michael J (Co-Principal)

Non-Syndromic Hearing Loss - A Collaborative Study
National Institutes of Health
R01DC002842
September 1, 2014 - August 31, 2019
Percent effort: 10
Smith, Richard (Principal Investigator), Schnieders, Michael J (Co-Investigator), Wang, Kai (Co-Investigator)

C3 Glomerulopathy - A Collaborative Study
National Institutes of Health
R01DK110023
April 1, 2017 - March 31, 2022
$1,967,814
Percent effort: 10
Smith, Richard J (Multi-PI), Nester, Carla M (Multi-PI), Schnieders, Michael J (Multi-PI), Breheny, Patrick J (Multi-PI)

Not Funded

Optimizing the accuracy of protein models associated with wild-type and mutated genes implicated in cancer
The University of Iowa Vice President for Research
January 1, 2015 - December 31, 2015
$27,208
Downing, Nancy R (Principal Investigator), Schnieders, Michael J (Co-Principal)

Collaborative Research: Simultaneous Prediction of Crystal Structure and Thermodynamics
National Science Foundation
June 1, 2013 - May 30, 2016
$648,268
Ren, Pengyu (Principal Investigator), Schnieders, Michael J (Co-Principal), Yang, Wei (Co-Principal)

High Performance Computing Opportunities for Personalized Medicine
Intel Corporation
June 2015 - May 2017

$389,290
Schnieders, Michael J (Co-Principal), Johnson, Hans (Co-Principal)

Micromechanics of Deformation in Flexible Organic Molecular Co-Crystals
National Science Foundation
June 1, 2015 - May 31, 2018
$474,723
Stevens, Lewis L. (Principal Investigator), Schnieders, Michael J (Co-Principal), Wurster, Dale (Co-Principal)

Protein Structure Refinement Using a Polarizable Force Field
National Institutes of Health
December 1, 2013 - November 30, 2018
$1,667,650
Schnieders, Michael J (Principal Investigator)

CAREER: Understanding the Structure, Thermodynamics and Solubility of Polymer Crystals Using High-Performance Computing
National Science Foundation
July 1, 2016 - June 30, 2021
$522,329
Schnieders, Michael J. (Principal Investigator)

Multi-scale mechanics of flexible organic co-crystals
National Science Foundation
July 1, 2016 - June 30, 2021
$500,000
Stevens, Lewis (Principal Investigator), Schnieders, Michael J (Co-Principal), Wurster, Dale (Co-Principal)

Understanding Highly Charged Molecular Recognition and Design Using Computation and Experiment
National Institutes of Health
July 1, 2016 - June 30, 2021
$1,607,288
Schnieders, Michael J (Principal Investigator), Fuentes, Ernesto (Principal Investigator)

The Role of ER Stress and Glaucoma
National Institutes of Health
May 1, 2018 - April 30, 2023
December 11, 2017
Percent effort: 10
Sheffield, Val C (Principal Investigator), Fingert, John H (Multi-PI), Scheetz, Todd E (Co-Investigator), Schnieders, Michael J (Co-Investigator)

Functional p53 mutants as predictors of response in ovarian cancer
National Institutes of Health
July 1, 2020 – 2025
$2,957,837
October 30, 2019
Percent effort: 8.3
Leslie, Kimberly K (Principal Investigator), Schnieders, Michael J (Co-Investigator)

Accelerating Missense variant interpretation through structural modeling and epistatic interactions
December 1, 2021 – November 31, 2024
$693,738
July 6, 2021
Percent effort: 20.0
Michelson, Jacob (Principal Investigator), Schnieders, Michael (Co-Investigator)

CleftProtein: Interpreting Cleft Lip and Palate Genetics Using AI and Simulation
July 1, 2021 – June 30, 2022
$291,017
May 14, 2021
Percent effort: 20.0
Butali, Azeez (Principle Investigator), Schnieders, Michael (Co-Investigator)

Building a Diverse Omics Workforce for Dental Oral and Craniofacial Research

December 1, 2022 – November 30, 2027
$1,592,472
January 19, 2022
Percent effort: 8.0
Butali, Azeez (Principle Investigator), Schnieders, Michael (Co-Investigator)

Fellowship

Funded

Donald D. Harrington Faculty Fellow
The University of Texas at Austin
September 2019 - May 2020
Percent effort: 100
Schnieders, Michael J (Principal Investigator)

D. Presentations

Conference Presentation

August 2015	Fall Meeting, American Chemical Society, Boston, Massachusetts United States. *Polarizable AMOEBA Free Energies at the Speed of Fixed Charge Force Fields: May the (Dual) Force Be With You.* Nessler, IJ, Park, J, Stephens, LL, Schnieders, MJ (Presenter).
March 2016	Annual Meeting, Biophysical Society, Los Angeles, California United States. *Protein Sequence Optimization with a Polarizable Force Field: Insights from PDZ Domains.* Schnieders, MJ.
March 2016	Spring Meeting, American Chemical Society, San Diego, California United States. *The Structure and Thermodynamics of Peptide Crystals from Simulations with a Polarizable Force Field.* Nessler, IJ, Schnieders, MJ (Presenter).
July 2019	Joint Tinker-Charmm Developer Meeting*,* Institut Pasteur, Paris, France*, GPU-Accelerated AMOEBA Thermodynamics Using a Monte Carlo Approach to Orthogonal Space Sampling*. Schnieders, MJ.
July 2019	Tinker Developer Meeting, Sorbonne University, Paris, France, *Algorithms in Force Field X You May Find Useful*, Schnieders, MJ.

October 2019 XtalPi Rational Solid Form Design Summit, Cambridge, Massachusetts United States. *Alchemical Free Energy Simulations with Advanced Force Fields to Predict the Structure, Stability, and Solubility of Organic Crystals*, Schnieders, MJ.

Poster

August 2013 65th Anniversary Biochemistry Retreat, Department of Biochemistry, The University of Iowa, Iowa City. *Computational approach to understanding solubility of organic crystals.* Park, J (Presenter), McClain, B (Author), Macikenas, D (Author), Schnieders, MJ (Author).

August 2013 65th Anniversary Biochemistry Retreat, University of Iowa, Department of Biochemistry, Iowa City. *Optimal placement of protein side-chains using a many-body potential: new beginnings for dead end elimination.* LuCore, SD (Presenter), Gao, S (Author), Lynn, AM (Author), Tollefson, WT A (Author), Schnieders, MJ (Author).

February 2014 Biophysical Society: 58th Annual Meeting, Biophysical Society, San Francisco. *Biomolecular structure refinement & prediction using dead-end elimination with a polarizable force field.* Schnieders, MJ (Presenter).

April 2014 Research Open House, College of Engineering, College of Engineering, The University of Iowa, Iowa City. *Organic crystal deposition thermodynamics via alchemical simulation.* Park, J (Presenter), Nessler, I (Author), McClain, B (Author), Schnieders, MJ (Author).

April 2014 Research Open House, College of Engineering, The University of Iowa, Iowa City. *Protein repacking under a many-body potential improves structures and yields biological insights.* LuCore, SD (Presenter), Powers, KT (Author), Gao, S (Author), Lynn, AM (Author), Tollefson, WT A (Author), Fenn, TD, Washington, MT (Author), Schnieders, MJ (Author). *Best Poster, Center for Bioinformatics and Computational Biology*

July 2014 Summer Undergraduate Research Conference, The University of Iowa, Iowa City. *Computational modeling and refinement of proteins implicated in deafness using a polarizable force field.* Tollefson, WT A (Presenter), Smith, R (Author), Schnieders, MJ (Author).

July 2014 Summer Undergraduate Research Conference, The University of Iowa, Iowa City. *Protein structure refinement of common cancer genes.* Corrigan, R (Presenter), Downing, N (Author), Schnieders, MJ (Author).

August 2014 Biochemistry Retreat, Department of Biochemistry, The University of Iowa, Iowa City. *Ensemble Refinement of Protein Crystal Structures.* Litman, J (Presenter), Sharma, G (Author), Schnieders, MJ. *Third Place, Graduate Poster Category*

August 2014 Biochemistry Retreat, Department of Biochemistry, The University of Iowa, Iowa City. *Organic crystal deposition thermodynamics vial alchemical simulation.* Park, J (Presenter), Nessler, I (Author), McClain, B (Author), Schnieders, MJ (Author).

February 2017 Annual Meeting, Biophysical Society, New Orleans, Louisiana United States. *Polarizable Amoeba Force Field Metadynamics With Minimization Predicts Missing Protein Loops.* Avdic, A, Tollefson, MR, Tatro, N, LuCore, SD, Litman, JM, Fenn, TD, Schnieders, MJ (Presenter).

April 2017 Spring Meeting, American Chemical Society, San Fransisco, California United States. *Toward polarizable AMOEBA thermodynamics at xed charge ef ciency using a dual force eld approach: Application to peptides and proteins.* Litman, JM, LuCore, SD, O'Connell, C, Schnieders, MJ (Presenter).

Seminar

September 2012 BME Graduate Seminar, University of Iowa, Iowa City, Iowa. *Applications of Computational Molecular Biophysics: Towards Personalized Medicine*.

September 2012 CBCB Advisory Board, University of Iowa, Iowa City, Iowa. *Computational Biophysics for Personalized Medicine*.

October 2012 Department of Biochemistry Workshop, University of Iowa, Iowa City, Iowa. *Applications of Computational Molecular Biophysics: Toward Personalized Medicine*.

October 2012 Iowa Microscopy Society, The Central Microscopy Research Facility, University of Iowa, Iowa City, Iowa. *Improving X-ray Crystal Structures: Toward CryoEM*.

October 2012 T32 Retreat, CBCB, University of Iowa, Iowa City, Iowa. *Molecular Biophysics for Personalized Medicine*.

December 2012 National Institute of Environmental Health Sciences, Research Triangle Park, North Carolina. *Pharmaceutical Applications of Computational Molecular Biophysics*.

June 2013 Structural Biology Interest Group, Department of Biochemistry, The University of Iowa, Iowa City. *New methods in rotamer optimization, protein residue pKa determination, and applications thereof.* LuCore, SD (Presenter), Schnieders, MJ (Author).

July 2013 Free energy calculations: Three decades of adventure in chemistry and biophysics, The Snowmass Biophysics Workshop Series, Snowmass, Colorado. *Free energy differences between vacuum, solvated & crystalline phases.* Schnieders, MJ (Presenter).

September 2013 20 years of PME: A symposium in honor of Tom Darden, Lee G Pedersen and Darrin York, American Chemical Society, Indianapolis, Indiana. *Protein structure refinement with a polarizable force field and PME.* Schnieders, MJ (Presenter).

October 2013 Rutgers University, New Brunswick, New Jersey. *Pharmaceutical Applications of Computational Molecular Biophysics*.

November 2013 Schrödinger, New York City, New York. *Free Energy Differences Between Vacuum, Solvated & Crystalline Phases*.

December 2013 BME Senior Design, Biomedical Engineering Department, The University of Iowa, Iowa City. *Protein side-chain pKas: the importance of atomic polarizability, conformational changes, and entropy.* LuCore, SD (Presenter), Schnieders, MJ (Author).

February 2014 Physical Chemistry Seminar Series, Chemistry Department (Hosted by Dr. Claudio Margulis). *Prediction of the Structure, Thermodynamics and Solubility of Organic Crystals.* Schnieders, MJ (Presenter).

February 2014	Genentech, San Francisco, California. *Crystal Sublimation and Solubility from Alchemical Simulations with a Polarizable Force Field Compared to Experiment*.
March 2014	Pharmacology Seminar Series, Pharmacology Department (Hosted by Dr. Lewis Stevens), Iowa City, Iowa. *Applications of Polarizable Force Fields to the Design of Small Molecule and Biologic Therapuetics.* Schnieders, MJ (Presenter).
May 2014	Biomedical Engineering Senior Design Day, Biomedical Engineering Department, The University of Iowa, Iowa City. *Pharmaceutical formulation software package: Organic crystal thermodynamics.* Park, J (Presenter), Schnieders, MJ (Author). *Best Senior Design Award*
May 2014	Free Energy Methods in Drug Design, Vertex Pharmaceuticals, Cambridge, Massachusetts. *Toward Molecular Design Using Many-Body Physics.* Schnieders, MJ (Presenter).
June 2014	Midwest Organic Solid State Chemistry Symposium XXIV, The University of Iowa, Iowa City. *Absolute crystal thermodynamics: Growth of the asymmetric unit into a crystal via alchemy.* Park, J (Presenter), Nessler, I, Schnieders, MJ. *Third Place in Oral Presentation Award*
June 2014	Midwest Organic Solid State Chemistry Symposium XXIV, The University of Iowa, Iowa City. *Absolute organic crystal thermodynamics: Growth of the asymmetric unit into a crystal via alchemy.* Schnieders, MJ (Presenter), Park, J (Author), Nessler, I (Author).
June 2014	Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride Science Research Center, Telluride, Colorado. *Many-Body Algorithms for Crystal Thermodynamics and Protein Structure Refinement.* Schnieders, MJ (Presenter).
June 2014	The University of Iowa, Department of Biochemistry, Iowa City, Iowa. *Protein Structure Refinement and Prediction with a Polarizable Force Field*. *Computational Biochemistry Workshop organized by Dr. Ernie Fuentes*
July 2014	École Polytechnique, Thomas Simonson, École Polytechnique, Paris France. *Crystal Thermodynamics and Protein Refinement with a Polarizable Force Field.* Schnieders, MJ (Presenter).
July 2014	Protein Electrostatics: A Satellite Meeting of EBEC 2014, EBEC Portugal. *Development and Applications of Polarizable Atomic Multipole AMOEBA Protein Electrostatics.* Schnieders, MJ (Presenter).
July 2014	The University of Iowa, Iowa Institute for Human Genetics, Iowa City, Iowa. *3D Protein Structures from Experiment and Computational Molecular Biophysics*. *IIHG short course on Bioinformatics organized by Dr. Tom Bair*
June 2015	Development and Deployment of Chemical Software for Advanced Potential Energy Surfaces, National Science Foundation, Telluride, Colorado United States. *Can Polarizable AMOEBA Thermodynamics Approach the Speed of Fixed Charge Force Fields.* Schnieders, MJ.

July 2015	Free energy calculations: Three decades of adventure in chemistry and biophysics, Snowmass, Colorado United States. *Simulation Methods to Understand Organic Crystal Thermodynamics.* Schnieders, MJ.
May 2016	Vertex Free Energy Workshop, Boston, Massachusetts United States. *Sampling Approaches That Accelerate Free Energy Calculations From Expensive Force Fields.* Schnieders, MJ.
June 2016	National Institutes of Health, Bethesda, Maryland United States. *Accelerating Polarizable Multipole Free Energy Calculations: Application to Organic Crystal Thermodynamics.* Schnieders, MJ.
July 2017	Free energy calculations: Three decades of adventure in chemistry and biophysics, Telluride, Iowa United States. *Chemical Theory for the "Protein Crystal Folding Problem".* Schnieders, MJ.
November 2019	Mitsubishi Tanabe Pharma, Tokyo, Japan, *Crystal Structure Prediction using Force Field X*. Schnieders, MJ.
November 2019	Yokohama City University, Tokyo, Japan, *Crystal Structure Prediction using Force Field X*. Schnieders, MJ.
November 2019	Hoshi University, Tokyo, Japan, *Crystal Structure Prediction using Force Field X*. Schnieders, MJ.
November 2019	Tokyo Institute of Technology, *Crystal Structure Prediction using Force Field X*. Schnieders, MJ.

IV. SERVICE

A. Memberships in Professional Organizations

2007 - Present	Biophysical Society
2012 - Present	American Chemical Society

B. Professional Service

2015 - 2016	Vertex 2016 Workshop on Free Energy Methods in Drug Design: Targeting Cancer, Workshop Organizer
2017 - 2018	2018 Workshop on Free Energy Methods, Kinetics and Markov State Models in Drug Design, Workshop Organizer
2012 - Present	Force Field X: Sustainable Software for Molecular Biophysics

C. University, College, Department Service

University

2016 - 2019	Genetics Cluster Steering Committee, Member
2015 - present	Research Computing Council, Member

College

2016 - 2018	Engineering Technology Committee, Member
2018 - 2019	Engineering Technology Committee, Chair
2019 - present	Iowa Institute for Artificial Intelligence Internal Advisory Board, Member

Department

2012 - 2014	BME Faculty Meeting Secretary, Officer, Secretary
2013 - 2014	BME Bioinformatics Search Committee, Member
2018 - 2019	BME Informatics Search Committee, Member
2013 - Present	BME Graduate Committee, Member
2013 - Present	BME Undergraduate Advisor (~16-18 students per year)

2021 - Present Biochemistry Graduate Recruiting Committee, Chair

D. Community Service

Relevant Public or Community Involvement

Local

2015 - Present West Liberty High School "*Science Club*" Program