Melisa Alkan

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Education and Training

Postdoctoral Scholar, Stanford University, Stanford, CA *Aug. 2023 - Present*
Department of Chemistry and the PULSE Institute, SLAC National Accelerator Laboratory
Advisor: Prof. Todd J. Martinez

Ph.D. in Theoretical Chemistry, Iowa State University, Ames, IA *Jul. 2018 – Jun. 2023*
Advisors: Prof. Mark S. Gordon, Prof. Levi M. Stanley
Thesis: "One programming model to rule them all: High-performance computational chemistry and applications via OpenMP offloading mode"

B.Sc. in Chemistry, Illinois Institute of Technology, Chicago, IL *Aug. 2014 – May 2018*
Advisors: Prof. Andrey Yu. Rogachev, Prof. Jean-Luc Ayitou

Research Experience

Ph.D. Researcher, Dr. Mark S. Gordon group, Iowa State University *2018 - 2023*

Development of a fragmentation library for accelerated quantum chemistry calculations in GAMESS

- Developed and implemented the Head-Gordon-Pople (HGP) algorithm and a novel digestion approach for the Hartree-Fock method via C++/CUDA programming models for scalable calculations on the pre-exascale supercomputer Summit targeting NVIDIA GPUs
- Achieved >80% parallel efficiency up to 1024 Summit nodes (6144 V100 GPUs) and a linear weak scaling up to 612 nodes for a 27,564-atom system

Development of a portable high-performance library for accelerated integral calculations

- Developed a GPU algorithm for two-electron integrals evaluation based on Rys-Quadrature and Rotated-axis scheme via Fortran/OpenMP offloading model
- Successfully ported the GPU-offloaded integrals to NVIDIA, AMD, and Intel GPUs
- Participated in an industry collaboration with NVIDIA to enable standard Fortran parallelism in GAMESS via "DO CONCURRENT" constructs and achieved 3x speedups in comparison to the current state-of-the-art parallel hybrid MPI/OpenMP code *(featured at NVIDIA GTC 2022)*

Ph.D. Researcher, Dr. Levi M. Stanley Group, Iowa State University *2018 - 2023*

Applications of computational chemistry to homogeneous catalysis

- Theoretically investigated the mechanism of a Pd-catalyzed carboacylation reaction via ester C-O bond activation
- Proposed a new nucleophile species for the reaction, which was experimentally confirmed
- Calculated mechanistic pathways for all plausible competing reactions and identified the lowest barrier pathway for the reported reaction

Grants and Fellowships

Molecular Software Science Institute (MolSSI) Fellowship *2022 - 2023*

- Secured independent funding for graduate tuition and research ($60k)

- One of 11 selected fellows in the United States to receive the fellowship for scientific software development

Brown Graduate Fellowship Award *2022 - 2023*
- One of 12 selected graduate students at Iowa State University to receive the fellowship ($10k) for research and career development

Awards and Recognitions

ISU Research Excellence Award *2023*
MIT PFPFEE Fellowship finalist *2023*
Klaus Ruedenberg Theoretical Chemistry Award *2022*
NVIDIA GPU award – competed at the national ACS conference and won an A30 GPU by NVIDIA *2022*
Chemistry Scholarship for Women *2021*
ISU Women in Chemistry Award *2019 and 2020*
ISU Teaching Excellence Award *2019*

Teaching and Mentoring

Mentoring students, Iowa State University *2021 - 2023*
- Mentored an undergraduate student in Prof. Mark S. Gordon's research group in a summer project
- Supervised two graduate students in Prof. Mark S. Gordon lab and one graduate student in Prof. Levi M. Stanley lab

Teaching Assistant, Iowa State University *2018 - 2019*
- General Chemistry II course – laboratory and teaching assistant
- Physical Chemistry thermodynamics course - laboratory and teaching assistant

Academic Resource Center (ARC) Scholar, Illinois Institute of Technology *2016 - 2018*
- Tutored and mentored students in undergraduate chemistry courses, including general chemistry I and II, organic chemistry I and II, analytical chemistry, instrumental analysis, physical chemistry I and II
- Served as a supplemental Instructor (SI) for General Chemistry I (CHEM124) and Organic Chemistry II (CHEM239) courses

Service and Outreach

Midwest Retreat for Diversity in Chemistry (MWRDC) Planning Committee Member *2020 - 2022*
- Planned and organized MWRDC retreat in Grinnell, IA with the mission to advance underrepresented groups in chemistry

American Society of Mechanical Engineers (ASME)-IIT invited panelist *2021*
- Participated in a career panel discussion for undergraduate students at Illinois Tech

Emmanuel College invited lecturer *2022*
- Taught a lecture on applications of machine learning in molecular modeling with a laboratory to 3rd and 4th year undergraduate students

Conference Presentations

Oral Presentations
- **M. Alkan** (presenter), G.M.J. Barca, J.L. Galvez-Vallejo, D.L. Poole, B. Pham, A.P. Rendell, M.S. Gordon "Development of new computer algorithms for heterogeneous architectures enable faster quantum chemistry calculations for reaction modeling", **The 2020 International Chemical Congress of Pacific Basin Societies (Pacifichem 2020),** Honolulu HI, Oral Presentation, 2021
- **M. Alkan** (presenter), A. Yu. Rogachev, "One- and three-electron bonding in conjugated hydrocarbons", **253th ACS National Meeting**, San Francisco CA, Oral Presentation, 2017

Poster Presentations

- **M. Alkan** (presenter), G.M.J. Barca, J.L. Galvez-Vallejo, D.L. Poole, B. Pham, A.P. Rendell, M.S. Gordon "Development of highly scalable multi-GPU quantum chemistry codes in GAMESS and applications to homogeneous catalysis", **ACS National Meeting 2022**, San Diego CA, NVIDIA Best GPU Poster Competition, 2022
- **M. Alkan** (presenter), H. K. Banovetz, Mark S. Gordon, Levi Stanley, "Merging theory and experiment: faster quantum chemistry calculations on GPUs for organic reactions", **The 2020 International Chemical Congress of Pacific Basin Societies (Pacifichem 2020),** Honolulu Hawaii, Poster Presentation, 2021
- **M. Alkan** (presenter), P. Xu, M.S. Gordon, "Many-Body Dispersion in Molecular Clusters", **255th ACS National Meeting**, New Orleans LA, Poster Presentation, 2018

Relevant Training Program

- MolSSI-Scientific Software Best Practices Workshop *2022*
- MolSSI-NVIDIA DLI Workshop on Fundamentals of Deep Learning (certified) *2022*
- Telluride School on Theoretical Chemistry (TSTC) *2021*
- Princeton GPU Hackathon by Oak Ridge National Lab, Princeton NJ *2020*
- ECP OpenMP Hackathon by SOLLVE, Atlanta GA *2020*
- Extreme Scale Computing training (ATPESC2020), Argonne National Laboratory *2020*

Publications

GPU offloading via Fortran/OpenMP

1. **M. Alkan**, T. Barnes, B. Pham, M.S. Gordon, "LibERI: A portable, performant, multi-GPU library for accelerated integrals calculations", *(in preparation),* 2023
2. **M. Alkan**, B. Pham, J.R. Hammond, M.S. Gordon, "Enabling standard Fortran parallelism in GAMESS", *Journal of Chemical Theory and Computation*, 2023, DOI: 10.1021/acs.jctc.3c00380
3. B. Pham, **M. Alkan**, M.S. Gordon, "Porting fragmentation methods to GPUs Using OpenMP API: offloading the Fock build for low angular momentum functions", *Journal of Chemical Theory and Computation*, 2023, DOI: 10.1021/acs.jctc.2c01137
4. **M. Alkan**, B. Chapman, B. Pham, C. Yang, C. Daley, C. Bertoni, D. Kulkarni, D. Oryspayev, E. D'Azevedo, J. Doerfert, K. Zhou, K. Ravikumar, M.S. Gordon, M. D. Ben, M. Lin, M. Kruse, O. Hernandez, P.K. Yeung, P. Lin, P. Xu, S. Pophale, T. Sattasathuchana, V. Kale, W. Huhn, and Yun (Helen) He, Outcomes of OpenMP Hackathon: OpenMP Application Experiences with the Offloading Model? (Part II), *Brookhaven National Lab. (BNL),* 2021, BNL-222064-2021-COPA

Accelerating QC calculations via C++/CUDA

5. G.M.J. Barca, **M. Alkan**, J.L. Galvez-Vallejo, D.L. Poole, A.P. Rendell, M.S. Gordon, "Faster Self-Consistent Field (SCF) Calculations on GPU Clusters", *Journal of Chemical Theory and Computation*, 2021, DOI: 10.1021/acs.jctc.1c00720
6. G.M.J. Barca, J.L. Galvez-Vallejo, D.L. Poole, **M. Alkan**, R. Stocks, A.P. Rendell, M.S. Gordon, Enabling large-scale correlated electronic structure calculations: scaling the RI-MP2 method on summit, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC'21), IEEE Press*, 2021, 40, 1-15, https://doi.org/10.1145/3458817.3476222
7. G.M.J. Barca, D.L. Poole, J.L. Galvez-Vallejo, **M. Alkan**, C. Bertoni, A.P. Rendell, M.S.Gordon, "Scaling the Hartree-Fock matrix build on summit", *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC'20), IEEE Press,* 2020, 81,1-14

Homogeneous Catalysis

8. **M. Alkan**, H.K. Banovetz, M.S. Gordon, L.M. Stanley, “Computational and mechanistic studies of Pd-catalyzed carboacylation reactions via ester C-O bond activation”, *ACS Catal.* 2023, 13, 14, 9766–9776. DOI: 10.1021/acscatal.3c01405
9. HK Banovetz, KL Vickerman, CM David, **M Alkan**, LM Stanley, Palladium-Catalyzed Intermolecular Alkene Carboacylation via Ester C–O Bond Activation, *Org. Lett.*, 2021, 23 (9), 3507-3512

Many-Body dispersion

10. P.Xu, **M.Alkan**, M.S.Gordon, “Many-Body Dispersion”, *Chemical Reviews,* 2020, DOI: 10.1021/acs.chemrev.0c00216
11. **M. Alkan**, P. Xu, M.S. Gordon, “Many-Body Dispersion in Molecular Clusters”, *J. Phys. Chem*. A, 2019, 123(39), 8406-8416. DOI: 10.1021/acs.jpca.9b05977

Materials for rechargeable batteries

12. H. Han, Z. Wei, A.S. Filatov, J.C. Carozza, **M. Alkan**, A.Yu. Rogachev, A. Svetsov, A. M. Abakumov, C. Park, M. Shatruk, Y. S. Cheng, E. V. Dikarev, “Three to tango requires a site-specific substitution: hetero tri metallic molecular precursors for high-voltage rechargeable batteries”, *Chem Sci*, 2019, 10, 524-534. DOI: 10.1039/C8SC03816C
13. A. Yu Rogachev, **M. Alkan**, J. Li, S. Liu, S. N. Spisak, A.S. Filatov, M.A. Petrukhina, “Mono-reduced Corannulene: To Couple and Not to Couple in One Crystal”, *Chem. Eur. J.*, 2019, 25, 14140-14147. DOI: 10.1002/chem.201902992
14. H. Han, Z. Wei, M.C. Barry, J.C. Carozza, **M. Alkan**, A. Yu. Rogachev, A.S. Filatov, A.M. Abakumov, and E.V. Dikarev, “A three body problem: a genuine heterotrimetallic molecule vs. a mixture of two parent heterobimetallic molecules”, *Chem. Sci.*, 2018, 9, 4736-4745. DOI: 10.1039/C8SC00917A
15. S.N. Spisak, A.V. Zabula, **M. Alkan**, A.S. Filatov, A. Yu. Rogachev, and M.A. Petrukhina, “Site-Directed Dimerizaition of Bowl-Shaped Radical Anions to Form a s-Bonded Dibenzocorannulene Dimer”, *Angew. Chem. Int. Ed.,* 2018, 57, 6171-6175. DOI: 10.1002/anie.201801537