Jon Paul Janet

Resumé

I am a scientist applying state-of-the-art machine learning techniques to solve challenging problems in early stage drug discovery at AstraZeneca. I am interested in how machine learning and computational chemistry can be combined to inform molecular design. My research has been featured in NeurIPS, Nature Machine Intelligence and various high-impact chemistry journals.

Experience

2022– **Associate Principal Scientist, Molecular AI**, AstraZeneca.
develop and apply generative reinforcement learning in combination with traditional structure- and ligand-based computational chemistry techniques to commercial early drug discovery projects. I also work with molecular property prediction, transformers for reaction informatics, active learning to close the gap between simulation and generative modeling, and generally evangelize around data-driven drug discovery!

2020–2022 **Senior Scientist, Computational Chemistry & Machine Learning**, AstraZeneca.

2015–2019 **Research Assistant, Machine Learning Materials Design**, Massachusetts Institute of Technology.
applied techniques from applied mathematics and machine learning combined with quantum chemical simulation for rational exploration and optimization in chemical space. Featured in MIT News a, ACS Chemical & Engineering News b, c and MIT Energy Futures d and authored a book titled Machine Learning in Chemistry as part of the ACS In Focus Series.

2018 **Teaching Assistant**, *Massachusetts Institute of Technology*.
graduate computational chemistry course at MIT, 6.8/7 student rating

2017 **Teaching Assistant**, *Singapore University of Technology and Design*.
second-year differential equations and optimization course for engineers

2014 **Internship, Computational Fluid Dynamics**, *Helmholtz-Zentrum Dresden-Rossendorf*.
investigated nucleation processes in dynamic 3D simulation of multiphase fluid flow

2013 **Research and Teaching Assistant**, *University of the Witwatersrand*.
designed and conducted experiments on biological remediation of acid mine drainage

Education

2015–2019 **Ph.D. Chemical and Computational Engineering**, *Massachusetts Institute of Technology*.

2014–2015 **M.Sc. Scientific Computing**, *Technical University of Berlin*.

2013–2014 **M.Sc. Applied Mathematics**, *Royal Institute of Technology, Stockholm*.

2009–2012 **B.Sc. Chemical Engineering (Hons.)**, *University of Cape Town*.

Skills and Projects

- **Programming** & **Machine learning**: Python, R, Matlab. Experienced with Pytorch, TensorFlow. Basic proficiency in C, MPI/high performance/parallel programming.
- **Computational Chemistry and simulation**: Experienced with quantum and classical simulation of molecular systems, dynamics, calculation automation and integration with machine learning, docking, free energy perturbation simulations.

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- **General**: Expert proficiency with LaTeX, TikZ, MS Office. Experienced with Linux, Windows & supercomputer administration, hardware and maintenance.
- **Open-source projects**:
  1. Core developer of molSimplify for 5 years – a python toolbox for inorganic molecular assembly and prediction. In particular, implemented the first neural-network assisted geometry initialization for quantum chemistry.
  2. Founder, core developer of molSimplify Automatic design – a python toolbox for combining simulation and machine learning for molecular design

Selected Publications

1. J. P. Janet, L. Mervin, and O. Engkvist. Artificial intelligence in molecular de novo design: Integration with experiment. *Current Opinion in Structural Biology*, 80:102575, 2023. doi: 10.1016/j.sbi.2023.102575 – link
2. D. Buterez, J. P. Janet, S. J. Kiddle, D. Oglic, and P. Liò. Graph neural networks with adaptive readouts. In A. H. Oh, A. Agarwal, D. Belgrave, and K. Cho, editors, *Advances in Neural Information Processing Systems*, 2022. doi: 10.48550/arXiv.2211.04952 – link
3. J. P. Janet. *Data-Driven Mapping of Inorganic Chemical Space for the Design of Transition Metal Complexes and Metal-Organic Frameworks*, chapter 7, pages 127–179. 2022. doi: 10.1021/bk-2022-1416.ch007 – link
4. J. Guo, F. Knuth, C. Margreitter, J. P. Janet, K. Papadopoulos, O. Engkvist, and A. Patronov. Link-invent: Generative linker design with reinforcement learning. *Digital Discovery*, 2023. doi: 10.1039/D2DD00115B – link
5. J. P. Janet, C. Duan, A. Nandy, F. Liu, and H. J. Kulik. Navigating transition-metal chemical space: Artificial intelligence for first-principles design. *Accounts of Chemical Research*, 54(3): 532–545, 2021. doi: 10.1021/acs.accounts.0c00686 – link
6. J. Guo, V. Fialková, J. D. Arango, C. Margreitter, J. P. Janet, K. Papadopoulos, O. Engkvist, and A. Patronov. Improving de novo molecular design with curriculum learning. *Nature Machine Intelligence*, 4(6):555–563, 2022. doi: 10.1038/s42256-022-00494-4 – link
7. J. P. Janet, C. Duan, A. Nandy, F. Liu, and H. J. Kulik. Navigating transition-metal chemical space: Artificial intelligence for first-principles design. *Accounts of Chemical Research*, 54(3): 532–545, 2021. doi: 10.1021/acs.accounts.0c00686 – link
8. J. P. Janet and H. J. Kulik. *Machine Learning in Chemistry*. American Chemical Society, Washington, DC, USA, 2020. doi: 10.1021/acs.infocus.7e4001 – link
9. S. M. Moosavi, A. Nandy, K. M. Jablonka, D. Ongari, J. P. Janet, P. G. Boyd, Y. Lee, B. Smit, and H. J. Kulik. Understanding the diversity of the metal-organic framework ecosystem. *Nature Communications*, 11(1):4068, Aug 2020. doi: 10.1038/s41467-020-17755-8 – link
10. J. P. Janet, S. Ramesh, C. Duan, and H. J. Kulik. Accurate multiobjective design in a space of millions of transition metal complexes with neural-network-driven efficient global optimization. *ACS Central Science*, 6(4):513–524, 2020. doi: 10.1021/acscentsci.0c00026 – link
11. J. P. Janet, C. Duan, T. Yang, A. Nandy, and H. J. Kulik. A quantitative uncertainty metric controls error in neural network-driven chemical discovery. *Chemical Science*, 10:7913–7922, 2019. doi: 10.1039/C9SC02298H – link
12. J. P. Janet, L. Chan, and H. J. Kulik. Accelerating chemical discovery with machine learning: Simulated evolution of spin crossover complexes with an artificial neural network. *The Journal of Physical Chemistry Letters*, 9(5):1064–1071, 2018. doi: 10.1021/acs.jpclett.8b00170 – link
13. A. Nandy, C. Duan, J. P. Janet, S. Gugler, and H. J. Kulik. Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry. *Industrial & Engineering Chemistry Research*, 57(42):13973–13986, 2018. doi: 10.1021/acs.iecr.8b04015 – link
14. J. P. Janet and H. J. Kulik. Resolving transition metal chemical space: Feature selection for machine learning and structure–property relationships. *The Journal of Physical Chemistry A*, 121(46):8939–8954, 2017. doi: 10.1021/acs.jpca.7b08750 – link
15. J. P. Janet and H. J. Kulik. Predicting electronic structure properties of transition metal complexes with neural networks. *Chemical Science*, 8:5137–5152, 2017. doi: 10.1039/C7SC01247K – link