Jon Paul Janet

Resumé

I use **machine learning** to solve challenging **real scientific problems** such as **discovering new materials using computational chemistry**. I am interested in how **data and simulation** can be combined to **inform design strategies**, and how to **quantify uncertainty in machine learning**.

Experience

Research

2015- **Research Assistant, Machine Learning Materials Design**, Massachusetts Institute of Technology.
combined computational chemistry and machine learning to design new materials[1–10].Featured in Chemical & Engineering News `https://cen.acs.org/articles/96/i8/Machine-learning-identifies-potential-inorganic.html`

2014 **Internship, Computational Fluid Dynamics**, *Helmholtz-Zentrum Dresden-Rossendorf.*
3D simulation of multiphase fluid flow[11]

2013 **Research and Teaching Assistant**, *University of the Witwatersrand.*
biological remediation of acid mine drainage[12]

2013 **Research Assistant**, *Process Modeling Group, University of Cape Town.*
designed reactor models for oil and gas processes

Teaching

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

2013 **Teaching Assistant**, *University of the Witwatersrand.*
first and second year chemical engineering core courses

2013 **Mathematics Tutor**, *Sum-It Maths.*
mathematics tutor for final year high school students

2010-2012 **Mathematics & Physics Tutor**, *Intuition Tutors.*
mathematics and physics tutor for final year high school students and university students

Education

2015–2019* **Ph.D. Chemical Engineering and Computation**, *Massachusetts Institute of Technology.*
quantum simulation, machine learning, materials design. *Ongoing

2014–2015 **M.Sc. Scientific Computing**, *Technical University of Berlin.*
control theory, DAE optimal control, model order reduction

2013–2014 **M.Sc. Applied Mathematics**, *Royal Institute of Technology, Stockholm.*
fluid mechanics, finite element methods, parallel programming

2009–2012 **B.Sc. Chemical Engineering (Hons.)**, *University of Cape Town.*
process design, transport, mathematics and modeling

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Skills and projects

- **Programming**: High proficiency: Python, R, Matlab. Basic proficiency: C, MPI/high performance/parallel programming.
- **Machine learning**: Experience designing and training neural networks and kernel models and uncertainty quantification. Experienced with TensorFlow, Keras and H2O frameworks.
- **Computational Chemistry and simulation**: Experienced with quantum and classical simulation of molecular systems, dynamics, calculation automation and integration with machine learning.
- **General**: Expert proficiency with LaTeX, TikZ, MS Office. Experienced with Linux, Windows & supercomputer administration, hardware and maintenance.
- **Open-source projects**:
  1. Principle maintainer, core developer of molSimplify – a python toolbox for inorganic molecular assembly and prediction (`https://github.com/hjkgrp/molSimplify`). Implemented the first neural-network assisted initialization for quantum chemistry
  2. Founder, core developer of molSimplify Automatic design – a python toolbox for combining quantum simulation and machine learning predictions for molecular design (`https://github.com/hjkgrp/AutomaticDesign`)
- Presented a workshop on machine learning in chemistry (`github.com/jpjanet/ML-chem-workshop`) at Ben Gurion University (02/14/19), Hebrew University of Jerusalem (02/17/19) and MIT (03/29/19).

Awards and Medals

- **Fellowships**: MIT-SUTD Graduate Fellow 2017, Erasmus Mundus Scholarship 2013–2015.
- **Awards**: MIT Center for Computational Engineering MathWorks Prize for doctoral research 2019, South African Institution of Chemical Engineers Silver Medal, City of Cape Town Engineering Medal, Malan Prize Overall Medal (all 2012). Chemical Engineering Class Medal 2012, 2011. Organic and Inorganic Chemistry Medal 2010. Dean's Merit List, 2009–2012.

Academic Publications

[1] J. P. Janet, A. Nandy, C. Duan, T. Yang, and H. Kulik. Uncertain times call for quantitative uncertainty metrics: Controlling error in neural network predictions for chemical discovery. *Submitted*, 2019. URL `https://chemrxiv.org/articles/Uncertain_Times_Call_for_Quantitative_Uncertainty_Metrics_Controlling_Error_in_Neural_Network_Predictions_for_Chemical_Discovery/7900277`.

[2] J. P. Janet, F. Liu, A. Nandy, C. Duan, T. Yang, S. Lin, and H. J. Kulik. Designing in the face of uncertainty: Exploiting electronic structure and machine learning models for discovery in inorganic chemistry. *Inorganic Chemistry, in press*, 2019.

[3] C. Duan, J. P. Janet, F. Liu, A. Nandy, and H. J. Kulik. Learning from failure: Predicting electronic structure calculation outcomes with machine learning models. *Journal of Chemical Theory and Computation, in press*, 2019.

[4] 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.

[5] 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.

[6] J. P. Janet and H. J. Kulik. Predicting electronic structure properties of transition metal complexes with neural networks. *Chemical Science*, 8:5137–5152, 2017.

[7] 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.

[8] J. P. Janet, T. Z. H. Gani, A. H. Steeves, E. I. Ioannidis, and H. J. Kulik. Leveraging cheminformatics strategies for inorganic discovery: Application to redox potential design. *Industrial & Engineering Chemistry Research*, 56(17): 4898–4910, 2017.

[9] A. Bajaj, J. P. Janet, and H. J. Kulik. Communication: Recovering the flat-plane condition in electronic structure theory at semi-local dft cost. *The Journal of Chemical Physics*, 147(19):191101, 2017.

[10] J. P. Janet, Q. Zhao, E. I. Ioannidis, and H. J. Kulik. Density functional theory for modelling large molecular adsorbate–surface interactions: a mini-review and worked example. *Molecular Simulation*, 43(5-6):327–345, 2017.

[11] J. P. Janet, Y. Liao, and D. Lucas. Heterogeneous nucleation in cfd simulation of flashing flows in converging–diverging nozzles. *International Journal of Multiphase Flow*, 74:106–117, 2015.

[12] J. P. Janet, K. Harding, C. Sheridan, and D. Drake. Increasing pumping depth in the long-term management of acid mine drainage. In *WISA 2014: Water Institute of Southern Africa*, South Africa, 2014.