

Victor Fung

Assistant Professor
School of Computational Science and Engineering
College of Computing
Georgia Institute of Technology

CODA TBD
Atlanta, GA 30308
Email: victorfung88@hotmail.com
Phone: 951-384-5242
Website: <https://www.fung-group.org/>

PROFESSIONAL EXPERIENCE

- 2022- **Assistant Professor**
School of Computational Science and Engineering, Georgia Institute of Technology
- 2019-2022 **Research Staff (Eugene P. Wigner Fellow)**
Nanomaterials Theory Institute, Oak Ridge National Laboratory
- 2015-2019 **Graduate Research Assistant**
Department of Chemistry, University of California Riverside
- 2018 **DOE Office of Science Graduate Student Research (SCGSR) Program Fellow**
Surface Chemistry and Catalysis Group, Oak Ridge National Laboratory
- 2014-2015 **Undergraduate Research Assistant**
Department of Chemistry and Chemical Biology, Cornell University

EDUCATION

- 2019 **Ph.D., Physical Chemistry**
University of California, Riverside (*advisor: Prof. De-en Jiang*)
- 2015 **B.A., Chemistry**
Cornell University (*advisor: Prof. Nandini Ananth*)

FELLOWSHIPS/AWARDS

- 2019 ORNL Eugene P. Wigner Fellow — Distinguished Staff Fellowship
Most prestigious fellowship currently offered at ORNL.
- 2019 UC Riverside Dissertation Year Program (DYP) Fellowship
- Nov 2018 Materials Research Society (MRS) Graduate Student Silver Award
- Aug 2018 American Chemical Society (ACS) COMP Division CCG Graduate Student Award
- June 2018 DOE Office of Science Graduate Student Research (SCGSR) Fellowship
UCR Today Highlight: <https://ucrtoday.ucr.edu/53035>
- 2015 UC Riverside Dean's Distinguished Fellowship

PUBLICATIONS ([Google scholar](#))

Total published articles/conference papers: **54**, Corresponding author: **7**, H-index: **25**, Citations: **1916**, (last updated 7/2022)

PREPRINTS:

- X1. Hülsey, M., **Fung, V.**, Yan, N., Hydrogen spillover and its relation to catalysis: observations on structurally defined single-atom sites (under revision) ([preprint](#))

PEER-REVIEWED ARTICLES (*denotes corresponding author):

52. Zachman, M., **Fung, V.**, Polo-Garzon, F., Cao, S., Moon, J., Huang, Z., Jiang, D., Wu, Z., Chi, M. "Measuring and directing charge transfer in heterogenous catalysts" Nature Communications 2022, 13, 1–8. ([link](#))
- 51.** **Fung, V.***, Ganesh, P., Sumpter, B.G., "Physically Informed Machine Learning Prediction of Electronic Density of States" Chem. Mater. 2022. ([link](#)) ([code](#))
50. Rosen, A. S., **Fung, V.**, Huck, P., O'Donnell, C. T., Horton, M. K., Truhlar, D. G., Persson, K. A., Notestein, J. M. & Snurr, R. Q. "High-Throughput Predictions of Metal–Organic Framework Electronic Properties: Theoretical Challenges, Graph Neural Networks, and Data Exploration." npj Comput. Mater. 2021, 8, 112 ([link](#))
49. Bao, Z., **Fung, V.**, Moon, J., Hood, Z., Rochow, M., Kammert, J., Polo-Garzon, F. and Wu, Z. *, "Revealing the interplay between "intelligent behavior" and surface reconstruction of non-precious metal doped SrTiO₃ catalysts during methane combustion" Catal. Today 2020. ([link](#))
- 48.** **Fung, V.***, Zhang, J.*, Hu, G., Ganesh, P., Sumpter, B.G., "Inverse design of two-dimensional materials with invertible neural networks" npj Comput. Mater. 2021, 7, 200. ([link](#)) ([code](#))
[Highlighted by ORNL: <https://www.ornl.gov/news/ornl-neural-network-study-harnesses-made-order-design-pair-properties-materials>]
47. Tang, Y., **Fung, V.**, Zhang, X., Li, Y., Nguyen, L., Sakata, T., Higashi, K., Jiang, D.E.*, Tao, F.F. *, "Single-Atom High-Temperature Catalysis on a Rh₁O₅ Cluster for Production of Syngas from Methane." J. Am. Chem. Soc. 2021, 143, 40, 16566–16579. ([link](#))
[Tang, Y.; **Fung, V.**; Zhang, X., Li, Y. share equal first author contribution]
- 46.** **Fung, V.***, Zhang, J., Juarez, E., Sumpter, B.G., "Benchmarking graph neural networks for materials chemistry." npj Comput. Mater. 2021, 7, 84. ([link](#)) ([code](#))
45. Luo, S., Li, M., **Fung, V.**, Sumpter, B.G., Liu, J., Wu, Z., Page, K., 2021. "New Insights into the Bulk and Surface Defect Structures of Ceria Nanocrystals from Neutron Scattering Study." Chem. Mater. 2021, 33, 11, 3959–3970. ([link](#))

44. Hu, G., **Fung, V.**, Huang, J., Ganesh, P., "Work Function Engineering of 2D Materials: The Role of Polar Edge Reconstructions"
J. Phys. Chem. Lett. 2021, 12, 9, 2320–2326. ([link](#))
43. Jiang, X., Sharma, L., **Fung, V.**, Park, S.J, Jones, C.W., Sumpter, B.G., Baltrusaitis, J., Wu, Z., "Oxidative Dehydrogenation of Propane to Propylene with Soft Oxidants via Heterogeneous Catalysts"
ACS. Catal. 2021, 11, 2182–2234. ([link](#))
42. Polo-Garzon, F.* , Blum, T., Bao, Z., Wang., K, **Fung, V.**, Huang, Z., Bickel, E., Jiang, D.E., Chi, M., Wu, Z., "In Situ Strong Metal–Support Interaction (SMSI) Affects Catalytic Alcohol Conversion"
ACS Catal. 2021, 11, 1938–1945. ([link](#))
- 41.** Zheng, X., Wei, K., Wang, Q., Kim, M., Sun, S., **Fung, V.***, Xia., X.* , "Nickel–Platinum Nanoparticles as Peroxidase Mimics with a Record High Catalytic Efficiency"
J. Am. Chem. Soc. 2021, 143, 7, 2660–2664. ([link](#))
[Highlights: ScienceDaily – <https://www.sciencedaily.com/releases/2021/03/210325120834.htm>;
Eurekalert – https://www.eurekalert.org/pub_releases/2021-03/uocf-nun032521.php]
- 40.** **Fung, V.***, Hu, G., Ganesh, P., Sumpter, B.G., "Machine Learned Features from Density of States for Accurate Adsorption Energy Prediction"
Nat. Commun., 2021, 12, 88. ([link](#)) ([code](#))
[Editor's highlight: www.nature.com/collections/ihbfhbiibg]
39. Cao, Y.; **Fung, V.**; Yao, Q.; Chen, T.; Zang, S.; Jiang, D. E.*; Xie, J. P.* "Control of Single-Ligand Chemistry on Thiolated Au₂₅ Nanoclusters"
Nat. Commun., 2020, 11, 5498. ([link](#))
38. **Fung, V.**; Hu, G.; Wu, Z.; Jiang, D.E.* , "Descriptors for Hydrogen Evolution on Single Atom Catalysts in Nitrogen-Doped Graphene"
J. Phys. Chem. C, 2020, 124, 19571–19578. ([link](#))
37. **Fung, V.**; Hu, G.; Wu, Z.; Jiang, D.E.* , "Hydrogen in Nanocatalysis"
J. Phys. Chem. Lett., 2000, 11, 17, 7049–7057. ([link](#))
36. Wang, K.; **Fung, V.**; Wu, Z.; Jiang, D.E.* , "Stable Surface Terminations of a Perovskite Oxyhydride from First Principles"
J. Phys. Chem. C, 2020, 124, 34, 18557–18563. ([link](#))
35. Polo-Garzon, F.; Blum, T.; **Fung, V.**; Bao, Z.; Chen, H.; Huang, Z.; Mahurin, S.; Dai, S.; Chi, M.; Wu, Z.* , "Alcohol-induced Low-Temperature Blockage of Supported-Metal Catalysts for Enhanced Catalysis"
ACS Catal., 2020, 10, 15, 8515–8523. ([link](#))

34. Wu, P., Tan, S., Moon, J., Yan, Z., **Fung, V.**, Li, N., Yang, S.Z., Cheng, Y., Abney, C.W., Wu, Z. Savara, A., Momen, A. M., Jiang, D. E, Su, D., Li, H., Zhu, W.* , Dai, S.* , Zhu, H.* , “Harnessing Strong Metal–Support Interactions via a Reverse Route.”
Nat. Commun., 2020, 11, 3042. ([link](#))
33. Kammert, J.; Moon, J.; Cheng, Y.; Daemen, L.; Irle, S.; **Fung, V.**; Liu, J.; Page, K.; Ma, X.; Phaneuf, V.; Tong, J.; Ramirez-Cuesta, A. J.; Wu, Z.* , “On the Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst”
J. Am. Chem. Soc., 2020, 142, 16, 7655–7667. ([link](#))
[Highlighted by BES: <https://www.energy.gov/science/bes/articles/novel-catalyst-means-ammonia-synthesis-less-heat-and-pressure>]
- 32.** Zhang, X.; You, R.; Wei, Z.; Jiang, X.; Yang, J.; Pan, Y.; Wu, P.; Jia, Q.; Bao, Z.; Bai, L.; Jin, M.; Sumpter, B.; **Fung, V.***; Huang, W.*; Wu, Z.* , “Radical Chemistry and Reaction Mechanisms of Propane Oxidative Dehydrogenation over Hexagonal Boron Nitride Catalysts”
Angew. Chem. Int. Ed., 2020, 59, 8042. ([link](#))
[Featured front cover: <https://onlinelibrary.wiley.com/doi/full/10.1002/anie.202004479>]
31. Hu, G.* , **Fung, V.**, Sang, X., Unocic, R. R., Ganesh, P.* , “Predicting Synthesizable Multi-Functional Edge Reconstructions in Two-Dimensional Transition Metal Dichalcogenides”
Npj Comput. Mater. 2020, 6, 44. ([link](#))
- 30.** **Fung, V.***, Hu, G., Sumpter, B.G., “Electronic Band Contraction Induced Low Temperature Methane Activation on Metal Alloys”
J. Mater. Chem. A 2020,8, 6057-6066. ([link](#))
29. Bao, Z.; **Fung, V.**; Polo-Garzon, F.; Hood, Z. D.; Cao, S.; Chi, M.; Bai, L.; Jiang, D. E.; Wu, Z.* , “The Interplay Between Surface Facet and Reconstruction on Isopropanol Conversion over SrTiO₃ Nanocrystals”
J. Catal. 2020, 384, 49-60. ([link](#))
28. Wan, Q.; **Fung, V.**; Lin, S.; Wu, Z.; Jiang, D. E.* Perovskite-Supported Pt single Atom for Methane Activation.
J. Mater. Chem. A, 2020, 8, 4362 – 4368. ([link](#))
27. Lee, K. H.; Vuong, V. Q.; **Fung, V.**; Jiang, D. E.; Irle, S.* , “Density-Functional Tight-Binding for Platinum Clusters and Bulk: Electronic vs Repulsive Parameters”
MRS Advances 2019, 4, 1821-1832. ([link](#))
26. Zheng, K.; **Fung, V.**; Yuan, X.; Jiang, D. E.; Xie, J. P.* "Real-time Monitoring of the Dynamic Intra-cluster Diffusion of Single Gold Atoms into Silver Nanoclusters"
J. Am. Chem. Soc., 2019, 141, 18977-18983. ([link](#))
[Featured front cover: https://pubs.acs.org/pb-assets/images/_journalCovers/jacsat/jacsat_v141i048-3.jpg]

25. Tian, C.; Zhang, H.; Zhu, X.*; Lin, B.; Liu, X.; Chen, H.; Zhang, Y.; Mullins, D. R.; Abney, C. W.; Shakouri, M.; Chernikov, R.; Hu, Y.; Polo-Garzon, F.; Wu, Z.; **Fung, V.**; Jiang, D. E.; Liu, X.; Chi, M.; Liu, J.; Dai, S.*, "A New Trick for an Old Support: Stabilizing Gold Single Atoms on LaFeO₃ Perovskite"
Appl. Catal. B., 2020, 261, 118178. ([link](#))
24. Hu, G.*; **Fung, V.**; Sang, X.; Unocic, R. R.; Ganesh, P.* "Superior Electrocatalytic Hydrogen Evolution at Engineered Non-Stoichiometric Two-Dimensional Transition Metal Dichalcogenide Edges."
J. Mater. Chem. A, 2019, 7, 18357-18364. ([link](#))
23. **Fung, V.**; Hu, G.; Tao, F.; Jiang, D.E.*, "Methane Chemisorption on Oxide-Supported Pt Single Atom"
ChemPhysChem, 2019, 20, 2217-2220. ([link](#))
22. Huang, R.; **Fung, V.**; Wu, Z.; Jiang, D.E.*, "Understanding the Conversion of Ethanol to Propene on In₂O₃ from First Principles"
Catal. Today, 2020, 350, 19-24. ([link](#))
21. Polo-Garzon, F.; **Fung, V.**; Nguyen, L.; Tang, Y.; Tao, F.; Cheng, Y.; Daemen, L. L.; Ramirez-Cuesta, A. J.; Foo, G. S.; Zhu, M.; Wachs, I. E.; Jiang, D. E.; Wu, Z.* "Elucidation of the Reaction Mechanism for High-Temperature Water-Gas Shift over an Industrially Relevant Copper-Chromium Iron Oxide Catalyst"
J. Am. Chem. Soc., 2019, 141, 7990-7999. ([link](#))
[Highlighted by Phys.org: <https://phys.org/news/2019-07-neutrons-industrial-catalyst-hydrogen-production.html>]
20. Tang, Q.; Hu, G.; **Fung, V.**, Jiang, D.E.*, "Insights into Interfaces, Properties, and Catalysis of Atomically Precise Metal Nanoclusters from First Principles"
Acc. Chem. Res., 2018, 51, 2793-2802. ([link](#))
19. **Fung, V.**, Wu, Z., Jiang, D.E.*, "New Bonding Model of Radical Adsorbate on Lattice Oxygen of Perovskites"
J. Phys. Chem. Lett., 2018, 9, 6321-6325. ([link](#))
18. Polo Garzon, F.; **Fung, V.**; Liu, X.; Bickel, E.; Bai, L.; Tian, H.; Foo, G. S.; Chi, M.; Jiang, D.E.; Wu, Z.* "Understanding the Impact of Surface Reconstruction of Perovskite Catalysts on CH₄ Activation and Combustion"
ACS Catal., 2018, 8, 10306-10315. ([link](#))
17. Chen, T.; **Fung, V.**; Yao, Q.; Luo, Z.; Jiang, D.E.; Xie, J.*, "Synthesis of Water-Soluble [Au₂₅(SR)₁₈]-using Stoichiometric Amount of NaBH₄"
J. Am. Chem. Soc., 2018, 140, 11370-11377. ([link](#))

16. Duchesne, P.; Li, Z.; Deming, C.; **Fung, V.**; Zhao, X.; Yuan, J.; Regier, T.; Aldalbahi, A.; Almarhoon, Z.; Chen, S.; Jiang, D. E.; Zheng, N.; Zhang, P. * "Golden Single-atomic-site Platinum Electrocatalysts"
Nat. Mater., 2018, 17, 1033-1039. ([link](#))
[*Li, Z.; Deming, C.; Fung, V. share equal second author contribution; Highlighted by Nature Middle East: <https://www.natureasia.com/en/nmiddleeast/article/10.1038/nmiddleeast.2018.118>*]
15. **Fung, V.**; Tao, F.; Jiang, D. E.* "Low-Temperature Activation of Methane on Doped Single Atoms: Descriptor and Prediction"
Phys. Chem. Chem. Phys., 2018, 20, 22909-22914. ([link](#))
14. Liu, J., **Fung, V.**, Wang, Y., Du, K., Zhang, S., Nguyen, L., Tang, Y., Fan, J., Jiang, D.E. and Tao, F.F.* "Promotion of Catalytic Selectivity on Transition Metal Oxide Through Restructuring Surface Lattice"
Appl. Catal. B., 2018, 237, 957-969. ([link](#))
[*Liu, J.; Fung, V. share equal first author contribution*]
13. Yao, Q. F.; **Fung, V.**; Sun, C.; Huang, S.; Chen, T.; Jiang, D. E.; Lee, J. Y.; Xie, J. P.* "Revealing Isoelectronic Size Conversion Dynamics of Metal Nanoclusters by a Noncrystallization Approach"
Nat. Commun., 2018, 9, 1979. ([link](#))
12. Huang, R.; **Fung, V.**; Zhang, Y.; Mullins, D. R.; Wu, Z.; Jiang, D. E.* "Understanding Methanol Coupling on SrTiO₃ from First Principles"
J. Phys. Chem. C, 2018, 122, 7210–7216. ([link](#))
11. Tang, Y.; Li, Y.; **Fung, V.**; Jiang, D. E.; Huang, W.; Zhang, S.; Iwasawa, Y.; Sakata, T.; Nguyn, L.; Zhang, X.; Frenkel, A.; Tao, F. F.* "Single Rhodium Atoms Anchored in Micropores for Efficient Transformation of Methane under Mild Condition"
Nat. Commun., 2018, 9, 1231. ([link](#))
[*Tang, Y.; Li, Y.; Fung, V. share equal first author contribution; Highlighted in C&EN News: <https://cen.acs.org/articles/96/web/2018/03/Catalyst-makes-acetic-acid-methane.html>*]
10. **Fung, V.**; Polo Garzon, F.; Wu, Z.; Jiang, D. E.* "Exploring Perovskites for Methane Activation from First Principles"
Catal. Sci. Tech., 2018, 8, 702-709. ([link](#))
[*Featured front cover: <http://pubs.rsc.org/en/content/articlepdf/2018/cy/c8cy90012d>*]
9. **Fung, V.**; Tao, F.; Jiang, D. E.* " Trends of Alkane Activation on Doped Cobalt (II, III) Oxide from First Principles"
ChemCatChem, 2018, 10, 244-249. ([link](#))
8. Yao, Q; Feng, Y.; **Fung, V.**; Yu, Y.; Jiang, D.E*; Yang, J.*; Xie, J.* "Precise Control of Alloying Sites of Bimetallic Nanoclusters via Surface Motif Exchange Reaction"

Nat. Commun., 2018, 8, 1555. ([link](#))

7. Yao, Q; Yuan, X.; **Fung, V.**; Yu, Y.; Jiang, D.E; Xie, J.* "Understanding Seed-Mediated Growth of Gold Nanoclusters: Hopping from One Stable Size to Another"
Nat. Commun., 2018, 8, 927. ([link](#))
6. Polo Garzon, F.; Yang, S.; **Fung, V.**; Chisholm, M. F.; Jiang, D. E.; Wu, Z.* "Controlling Reaction Selectivity via Surface Termination of Perovskite Catalysts"
Angew. Chem. Int. Ed., 2017, 56, 9820–9824. ([link](#))
[Highlighted by ScienceDaily: <https://www.sciencedaily.com/releases/2017/10/171018113508.htm>]
5. Foo, G. S.; Polo Garzon, F.; **Fung, V.**; Jiang, D.; Overbury, S.; Wu, Z.* "Acid-Base Reactivity of Perovskite Catalysts Probed via Conversion of 2-Propanol over Titanates and Zirconates"
ACS Catal., 2017, 7, 4423-4434. ([link](#))
4. **Fung, V.**; Tao, F.; Jiang, D.E.* "A General Structure-Reactivity Relationship for Oxygen on Transition Metal Oxides"
J. Phys. Chem. Lett., 2017, 8, 2206-2211. ([link](#))
3. **Fung, V.**; Jiang, D.E.* "Exploring Structural Diversity and Fluxionality of Pt_N (N=10-13) Clusters from First Principles"
J. Phys. Chem. C, 121, 2017, 10796-10802. ([link](#))
2. Liu, J.; Zhang, S.; Zhou, Y.; **Fung, V.**; Nguyen, L.; Jiang, D. E.; Shen, W. J.; Fan, J.; Tao, F. "Tuning Catalytic Selectivity on Metal Oxide through Deposition of Nonmetallic Atoms in Surface Lattice"
ACS Catal., 2016, 6, 4218-4228. ([link](#))
1. **Fung, V.**; Tao, F.; Jiang, D.E.* "Understanding Oxidative Dehydrogenation of Ethane on Co₃O₄ Nanorods from Density Functional Theory"
Catal. Sci. Tech., 2016, 6, 6861-6869. ([link](#))

CONFERENCE/WORKSHOP PUBLICATIONS:

2. Bi, S., **Fung, V.**, Zhang, J., Zhang, G., "Towards Efficient Uncertainty Estimation in Deep Learning for Robust Energy Prediction in Materials Chemistry" ICLR SimDL 2021 ([link](#))
1. Zhang, J., **Fung, V.**, "Efficient Inverse Learning for Materials Design and Discovery" ICLR SEDL 2021

PRESS/MEDIA COVERAGE

4. "AI for Materials Discovery" [Chemical & Engineering News](#), 2021
3. "Materials researchers put machine-learning performance to the test" [Chemical & Engineering News](#), April, 2021

2. "Early focus on sciences, happy accidents lead Wigner Fellow to career in computational chemistry" [ORNL News](#), January, 2020
1. "UCR Graduate Student Headed to Oak Ridge National Lab" [UCR Today](#), April 2018

PRESENTATIONS *invited talk

June 2022	*Seminar, Department of Chemistry, University of Tennessee, Knoxville, TN
May 2022	<i>Southeast Theoretical Chemistry Association (SETCA)</i> , Oral Presentation, Atlanta, GA
March 2022	<i>American Physical Society March Meeting</i> , Oral Presentation, Chicago, IL
Dec 2021	<i>Materials Research Society Fall Meeting</i> , Oral Presentation, Boston, MA
Nov 2021	* <i>AChE Annual Meeting</i> , Oral Presentation, Boston, MA
August 2021	<i>ACS 262nd National Meeting COMP Division</i> , Oral Presentation, Atlanta, GA
August 2021	* <i>Joint Nanoscience and Neutron Scattering User Meeting</i> , Oral Presentation, Oak Ridge, TN
June 2021	* <i>Telluride Computational Materials Chemistry Workshop</i> , Oral Presentation, Telluride, CO
May 2021	* <i>ORNL CNMS Seminar</i> , Oral Presentation, Oak Ridge, TN
March 2021	<i>RSCPoster</i> , Online
March 2020	<i>RSCPoster</i> , Online (2nd prize in Catalysis Division)
Feb 2020	* <i>ORNL ORPA Research Seminar</i> , Oral Presentation, Oak Ridge, TN
Feb 2020	* <i>Gordon Research Conference</i> , Discussion leader, Galveston, TX
Sept 2019	<i>18th Annual SE Catalysis Society Symposium</i> , Oral Presentation, Knoxville, TN
March 2019	<i>ACS 257th National Meeting CATL Division</i> , Oral Presentation, Orlando, FL
Feb 2019	<i>Gordon Research Seminar</i> , Oral Presentation, Ventura, CA <i>Gordon Research Conference</i> , Poster Presentation, Ventura, CA
Nov 2018	<i>Materials Research Society Fall Meeting</i> , Oral Presentation, Boston, MA
Sept 2018	<i>17th Annual SE Catalysis Society Symposium</i> , Oral Presentation, Atlanta, GA
Aug 2018	<i>ACS 256th National Meeting CATL Division</i> , Oral Presentation, Boston, MA <i>ACS 256th National Meeting COMP Division</i> , Poster Award Presentation, Boston, MA
May 2018	<i>3rd SoCal Theochem Symposium</i> , Poster Presentation, Pasadena, CA
March 2018	<i>UC Chemical Symposium 2018</i> , Oral Presentation, Lake Arrowhead, CA
March 2018	<i>ACS 255th National Meeting CATL Division</i> , Oral Presentation, New Orleans, LA
May 2017	<i>2nd SoCal Theochem Symposium</i> , Poster Presentation, Irvine, CA
April 2017	<i>Materials Research Society Spring Meeting</i> , Poster Presentation, Phoenix, AZ
April 2017	<i>ACS 253rd National Meeting COMP Division</i> , Oral Presentation, San Francisco, CA
Sept 2016	<i>2016 Pacific Coast Catalysis Society Meeting</i> , Poster Presentation, Riverside, CA
June 2016	<i>1st SoCal Theochem Symposium</i> , Poster Presentation, San Diego, CA
March 2016	<i>ACS 251st National Meeting CATL Division</i> , Oral Presentation, San Diego, CA

FUNDING/PROPOSALS

Funding:

10/2021-07/2022

PI: ORNL Laboratory Directed Research & Development

"Reinforced Adversarial Learning for Graph Generation and Design"

\$250K over one year

- 06/2021-06/2022 **Co-PI: ORNL Laboratory Directed Research & Development**
 "CO₂ Capture Mediated by Supramolecular Amine-Salt Network"
 \$190K over one year
- 09/2018 - 09/2020 **Co-PI: ORNL Laboratory Directed Research & Development**
 "Ammonia Synthesis Over 2D Electride-based Catalysts"
 \$968K over two years
- 05/2019 - 05/2021 **PI: ORNL Laboratory Directed Research & Development**
 "Using Fundamental Physicochemical Descriptors to Enable High-throughput Screening of Nanostructured Materials for New Energy Solutions"
 \$465K over three years

Resources:

- 01/2022 - 01/2023 **PI: NERSC DOE Mission Science Allocation**
 "Graph-based generative modelling for materials discovery and design"
 2390 CPU Node Hrs (956000 core hours); 750 GPU Node Hrs.
- 01/2021 - 01/2022 **PI: NERSC DOE Mission Science Allocation**
 "Exploration of Electronic Structure/Structure Space for High Throughput Materials Discovery with Machine Learning"
 520,000 CPU Hrs.
- 01/2020 - 01/2021 **PI: NERSC DOE Mission Science Allocation**
 "Machine Learned Features from Electronic Structure for High Throughput Materials Discovery"
 100,000 CPU Hrs.

TEACHING/SERVICE

Journal reviewer (manuscripts): Nature Catalysis (3), Nature Computational Science (1), Nature Communications (9), npj Computational Materials (3), Accounts of Chemical Research (1), Chemistry of Materials (1), Journal of Physical Chemistry Letters (1), Journal of Physical Chemistry C (1), Journal of Chemical Information and Modeling (1), ACS Applied Nano Materials (1), Small(1), Advanced Functional materials (1), Chemistry – A European Journal (1), Chemistry – Methods (1), ChemPhysChem (3), ChemistrySelect (2), Chemical Science (2), Physical Chemistry Chemical Physics (2), Journal of Materials Chemistry C (1), Catalysis Science and Technology (1), New Journal of Chemistry (1), RSC Advances (1), Molecular Catalysis (5), Applied Surface Science (2), Engineering – Elsevier (1), Chemical Engineering Science (1), AIP Advances (1), Physica B (1), MRS Advances (1), Matter(1), Cell Patterns (1), Computational Materials Science (1)

Conference reviewer:

International Catalysis Conference 2020

Proposal reviewer:

National Science Foundation, panel (2021)
 Swiss National Super Computing Center/ETH Zurich, ad hoc (2021)
 National Fund for Scientific and Technological Development, Chile, ad hoc (2020)

Conferences organized:

August 2021 *ACS 262nd National Meeting CATL Division, "Accelerating Catalysis Research with Machine Learning"*

May 2021 *SIAM MS21 Symposium, "Machine Learning for Solving Inverse Problems in Computational Chemistry and Materials Science"*

Mentorship:

2021-2022 *Pablo Unzueta, DOE SCGSR intern, UC Riverside PhD student*
2020- *Eric Juarez, SULI intern, Emory University BS student*
2018-2020 *Kristen Wang, UC Riverside PhD student*

Teaching/Service:

Nov 2018 *Materials Research Society Symposium Assistant, Boston, MA*
2017 *Graduate Teaching Assistant CHEM 001-A Lecture*
April 2017 *Materials Research Society Symposium Assistant, Phoenix, AZ*
2015-2016 *Graduate Teaching Assistant CHEM 001-LA Lab*
May 2016 *UC Riverside Chemistry Outreach STEM module, Riverside, CA*

Society Membership:

American Chemical Society, Materials Research Society, American Institute of Chemical Engineers

WEBSITES

Google Scholar	https://scholar.google.com/citations?user=2QsddMIAAAAJ&hl=en
LinkedIn	https://www.linkedin.com/in/victorxfung/
ResearchGate	https://www.researchgate.net/profile/Victor_Fung3
ORCID	https://orcid.org/0000-0002-3347-6983
GitHub	https://github.com/vxfung
Twitter	https://twitter.com/victorxfung
Personal website	https://www.fung-group.org