Victor Fung

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PROFESSIONAL EXPERIENCE

2019-	**Eugene P. Wigner Fellow** Nanomaterials Theory Institute, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
2018	**Department of Energy SCGSR Program Fellow** Chemical Sciences Division, Oak Ridge National Laboratory
2015-2019	**Graduate Research Assistant** Department of Chemistry, University of California Riverside
2014-2015	**Undergraduate Research Assistant** Department of Chemistry and Chemical Biology, Cornell University

EDUCATION

2019	**Ph.D. Physical Chemistry,** University of California Riverside
2015	**B.A. Chemistry,** Cornell University

FELLOWSHIPS/AWARDS

2019	ORNL Eugene P. Wigner Fellow — Distinguished Staff Fellowship
2019	UCR Dissertation Year Program Fellowship
Nov 2018	MRS Graduate Student Silver Award
Aug 2018	ACS COMP Division CCG Award
June 2018	DOE Office of Science Graduate Student Research (SCGSR) Fellowship
2015	UCR Dean's Distinguished Fellowship

PEER-REVIEWED JOURNAL PUBLICATIONS (Google scholar) *corresponding author

Total published: 44, First/Co-first author: **14**, Corresponding: **4**, H-index:19, Citations: 1140

44. Hu, G., **Fung, V.**, Jingsong, H., 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, XXX, 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, XXX, 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 (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 $SrTiO_3$ 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 $LaFeO_3$ 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.**; Zili, W.; Jiang, D.E.*, "Understanding the Conversion of Ethanol to Propene on In_2O_3 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 CH_4 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 $[Au_{25}(SR)_{18}]$- using Stoichiometric Amount of $NaBH_4$"
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. **Fung, V.**; Tao, F.; Jiang, D.E.* "Understanding Oxidative Dehydrogenation of Ethane on Co_3O_4 Nanorods from Density Functional Theory"
Catal. Sci. Tech., 2016, 6, 6861-6869. (link)

1. 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)

PEER-REVIEWED 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

1. Zhang, J., Fung, V., "Efficient Inverse Learning for Materials Design and Discovery" ICLR SEDL 2021

PRESS/MEDIA COVERAGE

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

March 2021 *2021 RSCPoster*, Online
March 2020 *2020 RSCPoster*, Online (2nd prize in Catalysis Division)
Feb 2020 **Gordon Research Conference*, Discussion leader, Galveston, TX
Sept 2019 *18th Annual SE Catalysis Society Symposium,* Oral Presentation, Knoxville, TN
March 2019 *ACS 257th National Meeting CATL Division,* Oral Presentation, Orlando, FL
Feb 2019 *Gordon Research Seminar,* Oral Presentation, Ventura, CA
Gordon Research Conference, Poster Presentation, Ventura, CA
Nov 2018 *Materials Research Society Fall Meeting,* Oral Presentation, Boston, MA
Sept 2018 *17th Annual SE Catalysis Society Symposium,* Oral Presentation, Atlanta, GA
Aug 2018 *ACS 256th National Meeting CATL Division,* Oral Presentation, Boston, MA
ACS 256th National Meeting COMP Division, Poster Award Presentation, Boston, MA
May 2018 *3rd SoCal Theochem Symposium,* Poster Presentation, Pasadena, CA
March 2018 *UC Chemical Symposium 2018,* Oral Presentation, Lake Arrowhead, CA
March 2018 *ACS 255th National Meeting CATL Division,* Oral Presentation, New Orleans, LA
May 2017 *2nd SoCal Theochem Symposium,* Poster Presentation, Irvine, CA
April 2017 *Materials Research Society Spring Meeting,* Poster Presentation, Phoenix, AZ
April 2017 *ACS 253rd National Meeting COMP Division,* Oral Presentation, San Francisco, CA
Sept 2016 *2016 Pacific Coast Catalysis Society Meeting,* Poster Presentation, Riverside, CA
June 2016 *1st SoCal Theochem Symposium,* Poster Presentation, San Diego, CA
March 2016 *ACS 251st National Meeting CATL Division,* Oral Presentation, San Diego, CA

TEACHING/SERVICE

Peer reviews: Nature Catalysis, Nature Communications, Accounts of Chemical Research, Chemical Science, Chemistry of Materials, Journal of Materials Chemistry C, Journal of Physical Chemistry C, Journal of Chemical Information and Modeling, Chemistry-Methods, Catalysis Science and Technology, New Journal of Chemistry, RSC Advances, Molecular Catalysis, Applied Surface Science, ACS Applied Nano Materials, AIP Advances, Physica B
Reviewer for conferences: ICC 2020

Conferences organized:
August 2021 *ACS 262nd National Meeting Symposium,* "Accelerating Catalysis Research with Machine Learning"
May 2021 *SIAM MS21 Symposium,* "Machine learning for solving inverse problems in computational chemistry and materials science"

Mentorship:
2020- *Eric Juarez*, SULI intern
2018-2020 *Kristen Wang*, UCR PhD student

Teaching:
2017 *Graduate Teaching Assistant CHEM 001-A Lecture*
2015-2016 *Graduate Teaching Assistant CHEM 001-LA Lab*
May 2016 *UC Riverside Chemistry Outreach STEM module,* Riverside, CA

WEBSITES

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