Peilin Liao

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ACADEMIC EXPERIENCE

2016 - Present	Assistant Professor, School of Materials Engineering, Purdue University
2014 - 2016	Postdoctoral Fellow, Department of Chemical & Biological Engineering, Northwestern University
2012 - 2014	Postdoctoral Research Scientist, Department of Chemistry, Columbia University
2012	Postdoctoral Research Associate, Department of Mechanical & Aerospace Engineering, Princeton University

EDUCATION

2012	Ph.D.	Princeton University, Princeton, NJ, USA Advisor: Emily A. Carter
2006	BSc	Peking University, Beijing, China

HONORS & AWARDS

2011	Graduate GPEC Solar Energy Innovation Award, Princeton University
2006 - 2010	Hugh Stott Taylor Fellowship, Princeton University
2007	David V. Milligan ’62 Fellowship, Princeton University
2006	Outstanding Graduate Award, Peking University

RESEARCH GRANTS

Current

1. “Computational Modeling of High Temperature Water-Gas Shift Reaction over Iron Oxide Catalysts,” P. Liao (PI); ACS Petroleum Research Fund (2018-2020)
2. “Integrated computational and experimental design of stable and defect-free semiconductors for solar cells: 2D perovskites and beyond,” P. Liao (PI), L. Dou & R. Agrawal, Purdue College of Engineering EFC seed grant 2019 Power, Energy, and the Environment (2019-2020)

PEER-REVIEWED PUBLICATIONS

Full list with citation metrics is available on Google Scholar and ResearcherID.

34. J. Shan, H. Wang, P. Yoo, L. Nguyen, F.-K. Chiang, S. Lee, **P. Liao**, J. Cheng, “Pt carbide nanomaterials and their catalytic applications in hydrocarbon conversion,” submitted.
33. Y. Poo and **P. Liao**,* “First principles study on hydrogen doping induced metal-to-insulator transition in rare earth nickelates $RNiO_3$ (R = Pr, Nd, Sm, Eu, Gd, Tb, Dy, Yb),” submitted.
32. J. Li, Z. Liu, D. A. Cullen, W. Hu, J. Huang, L. Yao, Z. Peng, **P. Liao**, R. Wang, “Distribution and valence state of Ru species on CeO_2 supports: support shape effect and its influence on CO oxidation,” ACS Catal., 9, 12, 11088 (2019). DOI: 10.1021/acscatal.9b03113.

31. S. Yao, Y. Poo, **P. Liao**,* "Computational study of hydrogen doping induced metal-to-insulator transition in $CaFeO_3$, $SrFeO_3$, $BaFeO_3$ and $SmMnO_3$," Phys. Chem. Chem. Phys., 21, 25397 (2019). DOI: 10.1039/C9CP04669K.
30. Y. Gao, E. Shi, S. Deng, S. B. Shiring, J. M. Snaider, C. Liang, A. Liebman-Peláez, P. Yoo, M. Zeller, B. W. Boudouris, **P. Liao**, C. Zhu, Y. Yu, B. M. Savoie, L. Huang, L. Dou, "Molecular engineering of organic-inorganic hybrid perovskites quantum wells," *Nat. Chem.*, 11, 1151 (2019). DOI: 10.1038/s41557-019-0354-2.
29. Y. Gao, Z. Wei, P. Yoo, E. Shi, M. Zeller, C. Zhu, **P. Liao**, L. Dou, "Highly stable lead-free perovskite field effect transistors incorporating linear pi-conjugated organic ligands,", *J. Am. Chem. Soc.*, 141, 15577 (2019). DOI: 10.1021/jacs.9b06276.
28. H. Zhu, H. Song, W. Zhao, Z. Peng, D. Liu, L. Xing, J. Dai, Z. Huang, **P. Liao**,* Y. Wang,* K. Wu,* "Chiral features of metal phthalocyanines sitting atop the pre-assembled TiOPc monolayer on Ag(111)," *Phys. Chem. Chem. Phys.*, 21, 16323 (2019). DOI: 10.1039/c9cp03198g.
27. S. T. Reeve, D. M. Guzman, L. Alzate-Vargas, B. Haley, **P. Liao**, A. Strachan, "Online simulation powered learning modules for materials science," *MRS Advances*, in press (2019). DOI: 10.1557/adv.2019.287.
26. H. Song, H. Zhu, Z. Huang, Y. Zhang, W. Zhao, J. Liu, Q. Chen, C. Yin, L. Xing, Z. Peng, **P. Liao**,* Y. Wang,* Y. Wang,* K. Wu,* "Steering the achiral into chiral of molecular orbital with a self-assembly strategy," *ACS Nano*, 13, 7202 (2019). DOI: 10.1021/acsnano.9b02683.
25. F. Song, W. Li, J. Yang, G. Han, T. Yan, X. Liu, Y. Rao,* **P. Liao,*** Z. Cao,* Y. Sun,* "Interfacial sites between cobalt nitride and cobalt act as superior bifunctional catalysts for hydrogen electrochemistry," *ACS Energy Lett.*, 4, 1594 (2019). DOI: acsenergylett.9b00738.
24. F. Song, W. Li, J. Yang, G. Han, **P. Liao**,* Y. Sun,* "Interfacing nickel nitride and nickel boosts both electrocatalytic hydrogen evolution and oxidation reactions," *Nat. Commun.*, 9, 4531 (2018). DOI: 10.1038/s41467-018-06728-7.
23. H. Chen,† **P. Liao**,† M. L. Mendonca,† R. Q. Snurr, "Insights into Catalytic Hydrolysis of Organophosphate Warfare Agents by Metal-Organic Framework NU-1000," *J. Phys. Chem. C*, 122, 12362 (2018). († denotes equal contribution) DOI: 10.1021/acs.jpcc.8b03641.
22. Y. Zhang, Y. Wang, **P. Liao**, K. Wang, Z. Huang, J. Liu, Q. Chen, J. Jiang, K. Wu, "Detection and Manipulation of Charge States for Double-Decker $DyPc_2$ Molecules on Ultrathin CuO Films," *ACS Nano*, 12, 2991 (2018). DOI: 10.1021/acsnano.8b00751.
21. S. Pellizzeri, M. Barona, V. Bernales, P. Miró, **P. Liao**, L. Gagliardi, R. Q. Snurr, R. B. Getman, "Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene," *Catal. Today*, 312, 149 (2018). DOI: 10.1016/j.cattod.2018.02.024.
20. P. Yoo and **P. Liao**,* "Metal-to-insulator transition in $SmNiO_3$ induced by chemical doping: a first principles study," *Mol. Syst. Des. Eng.*, 3, 264 (2018). DOI: 10.1039/C8ME00002F. (Part of the themed collection: MSDE Emerging Investigators 2018)
19. E. Argueta, J. Shaji, A. Gopalan, **P. Liao**, R. Q. Snurr, and D. A. Gomez-Gualdron, "Molecular building block-based electronic charges for high-throughput screening of MOFs for adsorption applications," *J. Chem. Theory Comput.*, 14, 365 (2018). DOI: 10.1021/acs.jctc.7b00841.
18. **P. Liao**, R. B. Getman, R. Q. Snurr, "Optimizing open iron sites in metal-organic frameworks for ethane oxidation: A first-principles study," *ACS Appl. Mater. Interfaces*, 9, 33484 (2017). DOI: 10.1021/acsami.7b02195.
17. Q. Chen, J. R. Cramer, J. Liu, X. Jin, **P. Liao**,* X. Shao,* K. V. Gothelf,* K. Wu,* "Steering on-surface reactions by a self-assembly approach," *Angew. Chem.*, 129, 1 (2017). DOI: 10.1002/ange.201700745.

16. J. Liu, X. Fu, Q. Chen, Y. Zhang, Y. Wang, D. Zhao, W. Chen, G. Q. Xu, **P. Liao**,* and K. Wu,* "Stabilizing surface Ag adatoms into tunable single atom arrays by terminal alkyne assembly," *Chem. Commun.*, 52, 12944 (2016). DOI: 10.1039/C6CC06444B.

Before August 2016

15. S. Kwon,† **P. Liao**,† P. C. Stair, and R. Q. Snurr, "Alkaline-earth metal-oxide overlayers on TiO_2: application toward CO_2 photoreduction," *Catal. Sci. Technol.*, 6, 7885 (2016). DOI: 10.1039/C6CY01661H. († denotes equal contribution)
14. Y. Zhang, **P. Liao**, J. Kan, C. Yin, N. Li, J. Liu, Q. Chen, Y. Wang, W. Chen, G. Q. Xu, J. Jiang, R. Berndt, and K. Wu, "Low-temperature scanning tunneling microscopy study on electronic properties of double-decker dypc$_2$ molecule at the surface," *Phys. Chem. Chem. Phys.*, 17, 27019 (2015). DOI: 10.1039/c5cp03925h.
13. J. E. Mondloch, M. J. Katz, W. C. Isley III, P. Ghosh, **P. Liao**, W. Bury, G. W. Wagner, M. G. Hall, J. B. DeCoste, G. W. Peterson, R. Q. Snurr, C. J. Cramer, J. T. Hupp, and O. K. Farha, "Destruction of chemical warfare agents using metal-organic frameworks," *Nature Materials*, 14, 512 (2015). DOI: 10.1038/NMAT4238.
12. C. X. Kronawitter, I. Zegkinoglou, S.-H. Shen, **P. Liao**, I. S. Cho, O. Zandi, Y.-S. Liu, K. Lashgari, G. Westin, J.-H. Guo, F. J. Himpsel, E. A. Carter, X. L. Zheng, T. W. Hamann, B. E. Koel, S. S. Mao, and L. Vayssieres, "Titanium incorporation into hematite photoelectrodes: theoretical considerations and experimental observations," *Energy Environ. Sci.*, 7, 3100 (2014). DOI: 10.1039/c4ee01066c.
11. **P. Liao** and E. A. Carter, "New concepts and modeling strategies to design and evaluate photo-electro-catalysts based on transition metal oxides," *Chem. Soc. Rev.*, 42, 2401 (2013). DOI: 10.1039/c2cs35267b.
10. F. Libisch, C. Huang, **P. Liao**, M. Pavone, E. A. Carter, "Origin of the energy barrier to chemical reactions to O_2 on Al(111): evidence for charge transfer not spin selection," *Phys. Rev. Lett.*, 109, 198303 (2012). DOI: 10.1103/PhysRevLett.109.198303.
9. **P. Liao**, J. A. Keith, E. A. Carter, "Water oxidation on pure and doped hematite (0001) surfaces: prediction of Co and Ni as effective dopants for electrocatalysis," *J. Am. Chem. Soc.*, 134 (32), 13296 (2012). DOI: 10.1021/ja301567f.
8. **P. Liao** and E. A. Carter, "Hole transport in pure and doped hematite," *J. Appl. Phys.*, 112, 013701 (2012). DOI: 10.1063/1.4730634.
7. **P. Liao** and E. A. Carter, "Optical excitations in hematite (α-Fe_2O_3) via embedded cluster models: a CASPT2 study," *J. Phys. Chem. C*, 115, 20795 (2011). DOI: 10.1021/jp206991v.
6. M. C. Toroker, D. K. Kanan, N. Alidoust, L. Isseroff, **P. Liao**, E. A. Carter, "First principles scheme to evaluate band edge positions in potential transition metal oxide photocatalysts and photoelectrodes," *Phys. Chem. Chem. Phys.*, 13, 16644 (2011). DOI: 10.1039/c1cp22128k.
5. **P. Liao** and E. A. Carter, "Testing variations of the GW approximation on strongly correlated transition metal oxides: Hematite (α-Fe_2O_3) as a benchmark," *Phys. Chem. Chem. Phys.*, 13, 15189 (2011). DOI: 10.1039/c1cp20829b.
4. **P. Liao**, M. C. Toroker, E. A. Carter, "Electron transport in pure and doped hematite," *Nano Letters*, 11, 1775 (2011). DOI: 10.1021/nl200356n.
3. **P. Liao** and E. A. Carter, "*Ab initio* DFT+U predictions of the shear response of iron oxides," *Acta Materialia*, 58, 5912 (2010). DOI: 10.1016/j.actamat.2010.07.007.
2. **P. Liao** and E. A. Carter, "*Ab initio* DFT+U predictions of tensile properties of iron oxides," *J. Mater. Chem.*, 20, 6703 (2010). DOI: 10.1039/c0jm01199a.
1. N. J. Mosey, **P. Liao**, E. A. Carter, "Rotationally invariant *ab initio* evaluation of Coulomb and exchange parameters for DFT+U calculations," *J. Chem. Phys.*, 129, 014103 (2008). DOI: 10.1063/1.2943142.

INVITED TALKS

2019 Apr Physical Chemistry Seminars, Chemistry, Purdue University, West Lafayette, IN; First principles investigation of chemistry in metal-organic frameworks and transition metal oxides.

2019 Apr ACS 2019 National Meeting, Symposium: Simulations of Materials & Processes for Energy Applications, Orlando, FL; Computational investigation of electrochemistry on surfaces and interfacial structures.

2019 Feb Inorganic Chemistry Seminars, Chemistry, Purdue University, West Lafayette, IN; First principles investigation of chemistry in metal-organic frameworks and transition metal oxides/nitrides.

2018 Oct MS&T 18, Symposium: Interfaces, Grain Boundaries and Surfaces from Atomistic and Macroscopic Approaches, Columbus, OH; Computational Study of Chemistry on Surfaces and Interfacial Structures.

2018 Aug Condensed Matter Seminars, Condensed Matter Seminars, Purdue University, West Lafayette, IN; First principles investigation of oxides for solar applications and electronic devices.

2018 May Chinese American Chemical Society Great Lakes Chapter 22nd Annual Conference, Abbott Park, IL; Challenges for Launching an Academic Career.

2017 Aug Telluride Workshop: Computational Materials Chemistry, Telluride, CO; Optimizing open Fe sites in metal-organic frameworks (MOFs) for ethane oxidation: A first-principles study.

2016 Dec Indiana University - Purdue University Indianapolis, Indianapolis, IN; Computational materials design for water splitting and CO_2 reduction on semiconductors.

2016 Mar Purdue University, West Lafayette, IN; Towards computational materials design for renewable energy technology and catalysis.

CONFERENCE CONTRIBUTIONS

2019 June 26th North American Catalysis Society Meeting, Chicago, IL; Computational study of electrochemistry on interfacial structures. (Talk)

2019 Apr ACS 2019 National Meeting, Orlando, FL; First principles investigation of metal-to-insulator transitions in rare earth nickelates induced by chemical doping. (Talk)

2019 Jan Electronic Materials and Applications 2019 (EMA 2019) Conference, Orlando, FL; First principles investigation of metal-to-insulator transitions in rare earth nickelates induced by chemical doping. (Talk)

2018 Nov MRS 2018 Fall Meeting, Boston, MA; First principles investigation of metal-insulator transitions in rare-earth nickelates induced by chemical doping. (Talk)

2018 July Gordon Research Conference: Solid State Chemistry, New London, NH; First principles investigation of metal-to-insulator transitions in rare earth nickelates ($RNiO_3$) induced by chemical doping. (Poster)

2018 June Gordon Research Conference: Catalysis, New London, NH; First principles study of Ni_3N/Ni interfaces for electrocatalytic hydrogen reactions & Fe inorganic nodes for C-H activation. (Poster)

2017 June 25th North American Catalysis Society Meeting, Denver, CO; Optimizing open Fe sites in metal-organic frameworks (MOFs) for ethane oxidation: A first-principles study.

2017 May Catalysis Club of Chicago 2017 Spring Symposium, Chicago, IL; Optimizing open Fe sites in metal-organic frameworks (MOFs) for ethane oxidation: A first-principles study. (Poster)

2016 May Catalysis Club of Chicago 2016 Spring Symposium, Chicago, IL; First-principles study of ethylene hydrogenation on transition metal oxide nanoclusters. (Poster)

2015 June 24th North American Catalysis Society Meeting, Pittsburgh, PA; First-principles study of chemical warfare agent decomposition on metal-organic frameworks. (Poster)

2012 May AFOSR Molecular Dynamics Program Review, Arlington, VA; First principles evaluation of optical, transport, and catalytic properties of pure and doped hematite for photocatalytic water splitting. (Poster)

2010 Oct Future Directions in CO_2 Conversion Chemistry Workshop, Princeton, NJ; Local and band-to-band excited states in hematite from quantum mechanics. (Poster)

2010 Aug Gordon Research Conference: Ceramics, New London, NH; Local and band-to-band excited states in hematite from quantum mechanics. (Poster)

2008 Aug ACS National Meeting, Division of Physical Chemistry, Philadelphia, PA; *Ab initio* evaluation of Coulomb (U) and exchange (J) parameters for DFT+U theory: Application to transition metal oxides.

2008 July American Conference on Theoretical Chemistry, Evanston, IL; *Ab initio* evaluation of Coulomb and exchange parameters for DFT+U theory: Application to transition metal oxides. (Poster)

2007 Nov Princeton Research Symposium, Princeton, NJ; First-principles calculations of iron oxides -- towards understanding of steel corrosion. (Poster)

CONFERENCE CONTRIBUTIONS – BY STUDENT ADVISEES

2019 June 26th North American Catalysis Society Meeting, Chicago, IL; Study on different surface terminations of Fe_3O_4 (111) for water-gas shift reaction with density functional theory (Pilsun Yoo,[G] Poster)

2019 June 26th North American Catalysis Society Meeting, Chicago, IL; First principles study of nickel nitride and nickel interface for electrocatalytic hydrogen evolution and oxidation reactions (Jiaqi Yang,[G] Poster)

2018 Oct 2018 AIChE Annual Meeting, Undergraduate Student Poster Competition, Pittsburgh, PA; Computational Catalysis: Creating a User-Friendly Tool for Research and Education (Kevin Greenman,[UG] Poster)

2018 Sept Frontiers of Molecular Engineering Meeting, Institute of Molecular Engineering, Chicago, IL; Composition effects on metal-to-insulator transition by chemical doping of rare earth nickelates $RNiO_3$ (R = Pr, Nd, Sm, Eu, Gd, Tb, Dy, Yb) (Pilsun Yoo,[G] Poster)

2018 Sept Frontiers of Molecular Engineering Meeting, Institute of Molecular Engineering, Chicago, IL; First principles study of nickel nitride and nickel interface for electrocatalytic hydrogen evolution and oxidation reactions (Jiaqi Yang,[G] Poster)

2018 May Catalysis Club of Chicago 2018 Spring Symposium, BP Research Center, Naperville, IL; First principles study of nickel nitride and nickel interface for electrocatalytichydrogen evolution and oxidation reactions (Jiaqi Yang,[G] Poster)

2018 Apr ASM Indianapolis April 2018 Chapter Meeting, Purdue University, West Lafayette, IN; First principle studies on chemical doping metal insulator transition of $SmNiO_3$ (Pilsun Yoo,[G] Poster)

PROFESSIONAL ACTIVITIES

2019 Reviewer for ACS Petroleum Research Fund

2019 Co-organizer & Session Chair: EAM 2019 symposium “Agile Design of Electronic Materials: Aligned Computational and Experimental Approaches and Materials Informatics”

2018 Reviewer for the 26th North American Catalysis Society Meeting

2017 Reviewer & Session Chair for the 25th North American Catalysis Society Meeting

Member of the Materials Research Society, Member of the American Ceramic Society, Member of the American Chemical Society

MANUSCRIPT REVIEWING

ACS: *J. Chem. Theory Comput.; J. Phys. Chem. C; Organometallics*

AIP: *Appl. Phys. Lett.; J. Chem. Phys.*

APS: *Phys. Rev. Lett.*

Elsevier: *J. Alloy Compd.; Computers & Chemical Engineering*

Nature Research: *Nat. Comm.*

IOP: *J. Phys. Condens. Matter*

RSC: *J. Mater. Chem.; Mater. Horiz.; Nanoscale; New J. Chem; Phys. Chem. Chem. Phys.; RSC Adv.; Catal. Sci. Technol.*

Springer: Theor. Chem. Acc.

Wiley: *Int. J. Quantum Chem.*

UNIVERSITY SERVICE

2019 - Present MSE Faculty Search Committee
2016 - Present MSE Graduate Admission Committee

TEACHING

2020 Spring	MSE597: Modeling & Simulation of Materials
2019 Fall	MSE270: Atomistic Materials Science
2019 Spring	MSE597: Modeling & Simulation of Materials
2018 Fall	MSE270: Atomistic Materials Science
2018 Spring	MSE270: Atomistic Materials Science
2017 Spring	MSE597: Modeling & Simulation of Materials

ONLINE EDUCATIONAL TOOLS DEVELOPMENT

8. A. N. Gentry[UG] & **P. Liao** (2020), "Introduction to Machine Learning in MSE: Predicting Bulk Modulus," https://nanohub.org/resources/msemlg. (DOI: 10.21981/4PNZ-RA03).
7. K. Greenman[UG] & **P. Liao** (2018), "Computational Catalysis with DFT," https://nanohub.org/resources/compcatal. DOI: 10.4231/D3PK0743B.
6. N. A. Miller[UG] & **P. Liao** (2018), "MSE educational tool: crystal structures, reciprocal lattice & symmetry," https://nanohub.org/resources/purduemse270. DOI: 10.4231/D38911T1R.
5. **P. Liao** (2017), "MSE educational tool: visualization of stacking faults," https://nanohub.org/resources/sfe. DOI: 10.4231/D38S4JR5Z.
4. **P. Liao** (2017), "MSE educational tool: elastic moduli calculations," https://nanohub.org/resources/elmod. DOI: 10.4231/D3280516X.
3. **P. Liao** (2017), "MSE educational tool: crystal structure and lattice plane visualization with Jmol," https://nanohub.org/resources/jmoltool. DOI: 10.4231/D3C824H0F.
2. **P. Liao** (2017), "MSE educational tool: X-ray diffraction (XRD) pattern," https://nanohub.org/resources/xrd. DOI: 10.4231/D3DJ58J8M.
1. G. Javier, U. Kamran, D. M. Guzman, A. Strachan, **P. Liao** (2017), "DFT Material Properties Simulator," https://nanohub.org/resources/dftmatprop. DOI: 10.4231/D30G3H12Q.

OUTREACH ACTIVITIES

Undergraduate mentoring

2018 May-Aug NCN Purdue Summer Undergraduate Research Fellowship (SURF) program
2017 May-Aug NCN Purdue Summer Undergraduate Research Fellowship (SURF) program

Outreach for K-12 grade students

2017 Apr NanoDays at Purdue 2017

STUDENT MENTORING

Graduate Advisees

Pilsun Yoo (2016 - Present), Jiaqi Yang (2017 - Present), Shukai Yao (2018 - Present)

Graduate Thesis Advisory Committee Member

Xiaohui Xu (MSE), Zachary McClure (MSE), Moonseop Kim (ME), Hong Sun (ME), Paulami Majumdar (ChemE), Ranga Rohit Seemakurthi (ChemE), Tianyi Li (ME), Pushkar G Ghanekar (ChemE), Licong An (MSE), Saswat Mishra (MSE), Nikhil Sharma (ME), Nicolae Iovanac (ChemE), Yinan Xu (ChemE), Aidan Coffey (ChemE)

Master Thesis Advisory Committee Member

Ram Kishore Venkatesan (ME)

Undergraduate Advisees

Abigail N Gentry (MSE), Nolan A Miller (MSE)