Yuan Ping
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Professional Preparation

University of Science and Technology of China	Chemical Physics	B.S. 2007
University of California, Davis	Theoretical Chemistry	Ph.D. 2013
California Institute of Technology	Materials Theory	Postdoctoral research, 2013-2016

Research Interests

Develop first-principles methods for excited states, spin dynamics, electronic transport in solid-state systems, quantum defects, and heterogenous interfaces for quantum information science and energy conversion applications. Specifically:

- Electronic excitation and exciton recombination from many-body perturbation theory
- Density matrix dynamics for open quantum systems and spin dynamics with quantum description of scatterings and many-body interactions
- Polaronic transport in doped metal oxides and perovskites

Appointments

July 2022-	Associate Professor, Department of Chemistry and Biochemistry, University of California, Santa Cruz
July 2016-	Assistant Professor, Department of Chemistry and Biochemistry, University of California, Santa Cruz
July 2017-	Affiliated Professor, Department of Physics, University of California, Santa Cruz
2013-2016	Materials Postdoctoral Fellow, Joint Center for Artificial Photosynthesis, California Institute of Technology (under supervision of Dr. William Goddard III)
2008-2013	Research Assistant, Department of Chemistry, University of California, Davis (under supervision of Dr. Giulia Galli)

Awards

- Alfred P. Sloan Research Fellow (2022)
- “Rising Talent” Speaker, American Conference on Theoretical Chemistry (2022)
- NSF CAREER Award (2022)
- ACS Open Eye COMP Award (2021)
- Air Force’s Young Investigator Award Program (YIP) (2021)
- Nature Research Award (shortlist) (2020)
- Journal of Materials Chemistry, *Emerging Investigator* (2019)
- Hellman Fellows (2018)

- Materials Postdoctoral Fellow (2013-2016)
- Travel award to Italy from Materials Computation Center at UIUC (2011)
- Outstanding Student Scholarship (2003–2006)

Grants

Grants as single PI or lead PI:

- DOE BES Computational Chemical Science Award, lead PI (9/1/2022-8/31/2025), $1.2M (Ping's share 618K), "Spin-Selective Photocatalysis and Quantum Transport using Ab-Initio Density-Matrix Dynamics" Award List

- NSF CAREER Award, Condensed Matter and Materials Theory (2022-2027), $555,274, "CAREER: Quantum Coherence, Optical Readout, and Quantum Transduction for Spin Qubits from First-Principles Calculations"

- Air Force's Young Investigator Research Program (YIP), single PI, (2021-2024), $450,000, "First-principles Spin Relaxation in Two-Dimensional Materials: Proximity, Twisting and Doping Effects"

- NSF, Condensed Matter and Materials Theory, lead PI, Grant No. DMR-1956015 (2020-2023), $497,627 (Ping's share 266K), "CDS&E: Ab Initio Ultrafast Dynamics of Spin, Valley and Charge in Quantum Materials"

- Alfred Sloan Research Fellowship (2022-2024), $75,000, "First-Principles Theory for Materials in Quantum Information Science"

- NSF Condensed Matter and Materials Theory, Single PI award, Grant No. DMR-1760260 (2018-2022), $353,130, "First-Principles Design of Charged Defects for Two-dimensional Quantum Technologies"

- Hellman Fellows (2019), $21,000

Grants as Co-PI/Senior personnel:

- DOE BES EFRC/CHOISE center, co-PI (thrust lead), (2022-2026), Ping's share $416,000, "Center for Hybrid Organic-Inorganic Semiconductors for Energy"

- NSF, Macromolec/Supramolec/Nano, co-PI, Grant No. CHE-2203633, (2022-2025), $526,000 (Ping: $250,000), "Chemical Control of Spin and Carrier Dynamics in 2D Hybrid Metal Halide Double Perovskites"

- NSF, Condensed Matter Physics, senior personnel, Grant No. DMR-2003563 (2020-2023), $532,227 (Ping: $180,000), "Mechanisms for Enhancing n-type Polaronic Transport in Transition Metal Oxides: Ionic size, Pair Formation/Clustering, and Valence Effects"

- NSF, Macromolec/Supramolec/Nano, co-PI, Grant No. CHE-1904547 (2019-2022), $449,886 (Ping: $150,000), "Understanding and Enhancing Electronic Coupling Between Metal Halide Perovskites Quantum Dots through Surface Molecular Engineering"

Students and Postdocs Mentored

Junqing Xu (postdoc, 2019-)
Hiroyuki Takenaka (postdoc, 2020-2022)
Feng Wu (postdoc, 2016-2019)
Tyler Smart (graduate student in physics, 2016-2021)
Chunhao Guo (graduate student in chemistry, 2018-)
Valentin Urena Baltazar (graduate student in chemistry, 2018-)
Kejun Li (graduate student in physics, 2019-)
Shiming Zhang (graduate student in physics, 2020-)
Andrew Grieder (graduate student in chemistry, 2021-)
Zachary Sanders-Bellis (undergraduate, 2018-2020)
Remi Leano (undergraduate, 2018-2019)
Anikeya Aditya (undergraduate, 2018-2019)

Publications

Google scholar: https://scholar.google.com/citations?user=w8iecRcAAAAJ&hl=en

Starting at UCSC:

Preprint:

62. "Substrate effects on spin relaxation in two-dimensional Dirac materials with strong spin-orbit coupling", Junqing Xu* and Yuan Ping*, *npj Computational Materials*, under review, (2022) preprint: https://arxiv.org/abs/2206.00784

61. "The Impacts of Dopants on the Small Polaron Mobility and Conductivity in Hematite – The Role of Disorder**",** Mingpeng Chen**,** Andrew C. Grieder**,** Tyler J. Smart**,** Kiley Mayford, Samuel NcNair, Anica Pinongcos, Samuel Eisenberg*,* Frank Bridges, Yat Li, and **Yuan Ping*,** under review, (2022).

60. "Strongly bound excitons reveal local spin chain directions in a van der Waals antiferromagnet", Dong Seob Kim, Di Huang, Chunhao Guo, Kejun Li, Dario Rocca, Frank Y. Gao, Jeongheon Choe, David Lujan, Edoardo Baldini, Li Yang, Shivani Sharma, Raju Kalivanan, Raman Shankar, Shang-Fan Lee, & **Yuan Ping***, and Xiaoqin Li*, under review, (2022). Underline authors are group members.

59. "Photocarrier induced persistent structural polarization in soft-lattice lead halide perovskites", Qi Qian, Zhong Wan, Hiroyuki Takenaka, Jong K Keum, Tyler J Smart, Laiyuan Wang, Peiqi Wang, Jingyuan Zhou, Huaying Ren, Dong Xu, Yu Huang, **Yuan Ping**, Xiangfeng Duan*, *Nature Nanotechnology*, under review, (2022). Underline authors are group members.

Peer-reviewed for all below:

58. "Nuclear spin polarization and control in a van der Waals material", Xingyu Gao, Sumukh Vaidya, Kejun Li, Peng Ju, Boyang Jiang, Zhujing Xu, Andres E. Llacsahuanga Allcca, Kunhong Shen, Takashi Taniguchi, Kenji Watanabe, Sunil A. Bhave, Yong P. Chen, **Yuan Ping**, and

Tongcang Li*, *Nature Materials,* in press, (2022). Underline authors are group members. DOI: https://doi.org/10.1038/s41563-022-01329-8

57. "Carbon Trimer as a 2 eV Single-Photon Emitter Candidate in Hexagonal Boron Nitride – A First-Principles Study"**,** Kejun Li, Tyler Smart, **Yuan Ping***, *Physical Review Materials (Letter),* 6, L042201, (2022). **Editor's suggestions.**

56. "Room-Temperature Electrically Switchable Spin-Valley Coupling in a van der Waals Ferroelectric Halide Perovskite with Persistent Spin Helix**"**, L. Zhang, J. Jiang, C. Multunas, C. Ming, Z. Chen, Y. Hu, Z. Lu, S. Pendse, R. Jia, M. Chandra, Y. Sun, T. Lu, **Y. Ping*,** R. Sundararaman*, J. Shi*, *Nature Photonics*, **16**, 529, (2022).

55. **"**Electric Field and Substrates Dramatically Accelerate Spin Relaxation in Graphene**",** A. Habib**,** J. Xu, **Y. Ping*** and R. Sundararaman***,** *Physical Review B***, 105**, 115122, (2022). preprint: arXiv:2012.11550 [cond-mat.mtrl-sci].

54. "The Critical Role of Synthesis Conditions on Small Polaron Carrier Concentrations in Hematite- A First-Principles Study"**,** Tyler Smart**,** Mingpeng Chen, Valentin Urena Baltazar**,** Frank Bridges, Yat Li, **Yuan Ping***, *Journal of Applied Physics*, **130**, 245705, (2021).

53. "Giant Spin Lifetime Anisotropy and Spin-Valley Locking in Silicene and Germanene from First-Principles Density-Matrix Dynamics", J. Xu, H. Takenaka, A. Habib, R. Sundararaman*, **Y. Ping***, *Nano Letters*, **21**, 9594, (2021).

52. "Ab initio Ultrafast Spin Dynamics in Solids**",** J. Xu, A. Habib, R. Sundararaman***** and **Y. Ping*,** *Physical Review B***, 104**, 184418, (2021). **Editor's Suggestions. Physics Magazine**

51. "Computational Design of Quantum Defects in Two-Dimensional Materials", **Y. Ping*** and T. Smart, *Nature Computational Science*, 1, 646, (2021). October Issue 2021 Journal Cover

50. "Approaching the intrinsic exciton physics limit in 2D semiconductor diodes**",** Peng Chen, Timothy L. Atallah, Zhaoyang Lin, Peiqi Wang, Sung-Joon Lee, Junqing Xu, Zhihong Huang, Xidong Duan, **Yuan Ping**, Yu Huang, Justin R. Caram,* Xiangfeng Duan*, *Nature*, in press, (2021). Underline authors are group members.

49. "Enhancing Defect Tolerance with Ligands at the Surface of Lead Halide Perovskites", T. Smart, H. Takenaka, T. Pham, L. Tan, J. Zhang*, T. Ogitsu*, and **Y. Ping***, *the Journal of Physical Chemistry Letters,* **12**, 6299, (2021).

48. "Doping Bottleneck in Hematite: Multipole Clustering by Small Polarons"**,** T. Smart, V. Baltazar, M. Chen, B. Yao, K. Mayford, F. Bridges, Y. Li, and **Y. Ping***, *Chemistry of Materials*, **33**, 4390, (2021).

47. "Substrate Effect on Excitonic Shift and Radiative Lifetime of Two-Dimensional Materials", C. Guo, J. Xu, and **Y. Ping***, *Journal of Physics: Condensed Matter*, **33,** 234001, (2021), Emerging leaders issue, preprint: arXiv:2101.00185 [cond-mat.mtrl-sci], (2021).

46. "Intersystem Crossing and Exciton-Defect Coupling of Spin Defects in Hexagonal Boron Nitride", T. Smart, K. Li, J. Xu, **Y. Ping***, *npj Computational Materials,* **7***,* 59, (2021)*,* preprint: arXiv:2009.02830 [cond-mat.mtrl-sci] (2020).

45. "High-order superlattices by rolling up van der Waals heterostructures", Bei Zhao, Zhong Wan, Yuan Liu, Junqing Xu,.. Chunhao Guo, ...Yu Huang, **Yuan Ping**, Xidong Duan and Xiangfeng Duan, *Nature,* 591, 385, (2021). Underline authors are group members.

44. "Organically Capped Iridium Nanoparticles as High-Performance Bifunctional Electrocatalysts for Full Water Splitting in Both Acidic and Alkaline Media: Impacts of Metal-Ligand Interfacial Interactions", Y. Peng, Q. Liu, B. Lu, T. He, F. Nichols, X. Hu, T. Huang, G. Huang, L. Guzman, **Y. Ping***, Shaowei Chen*, *ACS Catalysis*, **11**, 1179, (2021).

43. "Interplay between Perovskite Magic-Sized Clusters and Amino Lead Halide Molecular Clusters", E. Vickers, Z. Chen, V. Cherrette, T. Smart, P. Zhang, **Y. Ping**, and J. Zhang*, *Research - A Science Partner Journal*, 6047971, (2021).

42. "Substrate Screening Approach for Quasi-particle Energies of Lattice-mismatched Two-dimensional Interfaces", C. Guo, J. Xu, D. Rocca, **Y. Ping***, *Physical Review B*, **102**, 205113, (2020), **Editors' Suggestions.**

41. "Spin-phonon Relaxation from a Universal Ab initio Density-matrix Approach", J. Xu†, A. Habib†, S. Kumar, F. Wu, R. Sundararaman*, and **Y. Ping***, *Nature Communications*, **11**, 2780, (2020). UCSC News ScienceDaily Phys.Org

40. **"**Oxygen Reduction Reaction Catalyzed by Carbon-supported Platinum Few-atom Clusters: Significant Enhancement by Doping of Atomic Cobalt**",** B. Lu**,** Q. Liu, F. Nichols, R. Mercado, D. Morris, N. Li, P. Zhang, P. Gao, **Y. Ping** and S. Chen*, *Research*, 9167829, (2020).

39. "Interstitial Lithium Doping in $BiVO_4$ Thin Film Photoanode for Enhanced Solar Water Activity", C. Zhou, Z. Sanders-Bellis, T. Smart, W. Zhang, L. Zhang, **Y. Ping*** and M. Liu*, *Chemistry of Materials*, **32***,* 6401, (2020).

38. "Electrochemical Oxidation of Metal-Catechol Complexes as a New Synthesis Route to the High-Quality Ternary Photoelectrodes: A Case Study of Fe_2TiO_5 Photoanodes", D. Lee†**,** V. Baltazar†, T. Smart, **Y. Ping***; K. Choi*, *ACS Applied Materials & Interfaces*, **12**, 29275, (2020).

37. "Combined Experimental and Theoretical Investigations of n-Type $BiFeO_3$ for Use as a Photoanode in a Photoelectrochemical Cell"**,** A. Radmilovic†, T. Smart†, **Y. Ping***, K. Choi*, *Chemistry of Materials*, **32**, 3262, (2020).

36. ''The Coupling of Experiments with Density Functional Theory in the Studies of the Electrochemical Hydrogen Evolution Reaction", M. Chen, T. Smart, S. Wang, T. Kou, D. Lin, **Y. Ping*** and Y. Li*, *Journal of Materials Chemistry A*, **8**, 8783, (2020).

35. "Carbon Doping Switching on the Hydrogen Adsorption Activity of NiO for Hydrogen Evolution Reaction**"**, T. Kou†, M. Chen†**,** F. Wu, T. Smart, S. Wang, Y. Wu, Y. Zhang, S. Li, S. Lall, Z. Zhang, Y. Liu, J. Guo, G. Wang*, **Y. Ping***, and Y. Li*, *Nature Communications*, **11,** 590, (2020).

34. "Nanowrinkled Carbon Aerogels Embedded with FeN Sites as Effective Oxygen Electrodes for Rechargeable Zinc-Air Battery", T. He, B. Lu, Y. Chen, Y. Wang, Y. Zhang, J. Davenport, A. Chen, C. Pao , M. Liu, Z. Sun, A. Stram, A. Mordaunt, J. Velasco Jr., **Y. Ping**, Y. Zhang*, and S. Chen*, *Research – A Science Partner Journal,* **2019***,* 6813585 (2019).

33. “Oxygen Reduction Reaction Catalyzed by Black Phosphorus-Supported Metal Nanoparticles: Impacts of Interfacial Charge Transfer”, Y. Peng, B. Lu, N. Wang, J. Lu, C. Li*, **Y. Ping**, S. Chen*, *ACS Applied Materials and Interfaces*, **11**, 24707 (2019).

32. “Optical Absorption Induced by Small Polaron Formation in Transition Metal Oxides – The Case of Co_3O_4”, T. Smart**,** T. Pham, **Y. Ping***, and T. Ogitsu*, *Physical Review Materials (Rapid Communications)*, **3**, 102401(R), (2019).

31. “Carrier Recombination Mechanism at Defects in Wide Band Gap Two-dimensional Materials from First principles”, F. Wu, T. Smart, J. Xu, **Y. Ping***, *Physical Review B (Rapid Communication)*, **100**, 081407(R) (2019).

30.“Dimensionality and Anisotropicity Dependence of Radiative Recombination in Nanostructured Phosphorene”, F. Wu, D. Rocca and **Y. Ping***, *Journal of Materials Chemistry C*, **7**, 12891, (2019), invited paper in Emerging Investigators issue.

29. “Combined Theoretical and Experimental Investigations of Atomic Doping to Enhance Photon Absorption and Carrier Transport of $LaFeO_3$ Photocathodes”**,** G. Wheeler**†**, V. Baltazar**†,** T. Smart, A. Radmilovic, **Y. Ping***, and K. Choi*, *Chemistry of Materials*, **31**, 5890, (2019).

28. “Fundamental Principles for Calculating Charged Defect Ionization Energies in Ultrathin Two-Dimensional Materials”, T. Smart, F. Wu, M. Govoni and **Y. Ping*****, *Physical Review Materials,* **2**, 124002, (2018).

27. “Spin-optotronic Properties of Organo-metal Halide Pervoskites”, **Y. Ping*** and J. Zhang*, *Journal of Physical Chemistry Letter*, (invited), **9**, 6103, (2018).

26. “Combining Landau-Zener Theory and Kinetic Monte Carlo Sampling for Small Polaron Mobility of Doped BiVO4 from First-principles”, F. Wu and **Y. Ping*****, *Journal of Materials Chemistry A*, **6**, 20025, (2018).

25. “The Role of Point Defects in Enhancing the Conductivity of $BiVO_4$”, H. Seo, **Y. Ping** and G. Galli*, *Chemistry of Materials*, **30**, 7793, (2018).

24. “Mechanistic Insights of Enhanced Spin Polaron Conduction in CuO through Atomic Doping”, T. Smart**,** A. Cardiel**,** F. Wu**,** K. Choi and **Y. Ping*****, *npj Computational Materials*, **4**, 61, (2018).

23. “Unconventional Relation Between Charge Transport and Photocurrent via Boosting Small Polaron Hopping for Photoelectrochemical Water Splitting”, W. Zhang, F. Wu, J. Li, D. Yan, J. Tao, **Y. Ping** and M. Liu*, *ACS Energy Letters*, **3**, 2232, (2018).

22. “Ruthenium Atomically Dispersed in Carbon Outperforms Platinum toward Hydrogen Evolution in Alkaline Media”, B. Lu, L. Guo, F. Wu, Y Peng, J. Lu, T. Smart, Y. N. Wang, Y. Finfrock, D. Morris, P. Zhang, **Y. Ping*** and S. Chen*, *Nature Communications,* **10**, 631, (2018). (Hightlighted in News of ScienceDaily) (UCSC News)

21. “Point of Anchor: Impacts on Interfacial Charge Transfer of Metal Oxide Nanoparticles", Y. Peng, B. Lu, F. Wu, F. Zhang, J. Lu, X. Kang, **Y. Ping*** and S. Chen*, *Journal of the American Chemical Society*, **140**, 15290, (2018).

20. "Theoretical and Experimental Insight into the Effect of Nitrogen Doping on Hydrogen Evolution Activity of Ni_3S_2 in Alkaline Medium", T. Kou, T. Smart, B. Yao, I. Chen, D. Thota, **Y. Ping***, Y. Li*, *Advanced Energy Materials*, **8**, 1703538 (2018).

19. "First-principles Engineering of Charged Defects for Two-dimensional Quantum Technologies", W. Feng, A. Galatas A., R. Sundararaman, D. Rocca, and **Y. Ping*,** *Physical Review Materials* **1***,* 071001(R), (2017).

18. "Nitrogen and Iron-Codoped Carbon Hollow Nanotubules as High-Performance Catalysts toward Oxygen Reduction Reaction: A Combined Experimental and Theoretical Study"**,** B. Lu**,** T. Smart**,** D. Qin, J. Lu, N. Wang, Li. Chen, Y. Peng, **Y. Ping**[*] and S. Chen[*], *Chemistry of Materials*, **29**, 5617, (2017) ("Top 20 downloaded paper in Chemistry of Materials" in 2017)

17. "Hydrogen evolution reaction catalyzed by ruthenium ion-complexed graphitic-like carbon nitride nanosheets"**,** Y. Peng, B. Lu, L. Chen, N. Wang, J. Lu, **Y. Ping*** and S. Chen*, *Journal of Materials Chemistry A,* **5**, 18261, (2017)

16. "Effects of Defects on the Small Polaron Formation and Transport Properties of Hematite from First-Principles Calculations", T. Smart, and **Y. Ping***, *Journal of Physics Condensed Matter,* **29,** 394006, (2017).

15**.** "First-principles Electrostatic Potentials for Reliable Alignment at Interfaces and Defects", R. Sundararaman* and **Y. Ping*,** *The Journal of Chemical Physics***, 146,** 104109 (2017).

14. "The Reaction Mechanism with Free Energy Barriers at Constant Potentials for the Oxygen Evolution Reaction at the IrO_2 (110) Surface", **Y. Ping***, R. Nielsen, W. A. Goddard III*, *Journal of the American Chemical Society*, **139**, 149-155, (2017).

13. "Modeling Heterogeneous Interfaces for Solar Water Splitting", T. Pham*, **Y. Ping*** and G. Galli*, *Nature Materials*, **16**, 401, (2017).

<u>Before UCSC:</u>

12. "Electronic Structure of IrO_2: the Role of the Metal d Orbitals", **Y. Ping***, G. Galli and W. Goddard III*, *Journal of Physical Chemistry C*, **119**, 11570, (2015).

11. "Energetics and Solvation Effects at the Photoanode/Catalyst Interface: Ohmic Contact versus Schottky Barrier ", **Y. Ping***, W. Goddard III* and G. Galli, *Journal of the American Chemical Society*, **137**, 5264, (2015).

10. "Simultaneous Enhancements in Photon Absorption and Charge Transport of $BiVO_4$ Photoanodes for Solar Water Splitting", T. Kim, **Y. Ping**, G. Galli* and K. Choi*, *Nature Communications,* **6**, 8769, (2015). (Highlighted in News of University of Chicago)

9. "Solvation Effect on Band Edge Positions of Photocatalysts from First Principles", **Y. Ping*,** R. Sundararaman, and W. Goddard III, *Physical Chemistry Chemical Physics*, 2015, DOI: 10.1039/c5cp05740j. (Highlighted in the feature article of Joint Center for Artificial Photosynthesis)

8. “Optimizing the Band Edges of Tungsten Trioxide for Water Oxidation: a First Principles Study”, **Y. Ping*** and G. Galli, *Journal of Physical Chemistry C*, **118**, 6019, (2014).

7. “Electronic Excitations in Light Absorbers for Photoelectrochemical Energy Conversion: First Principles Calculations Based on Many Body Perturbation Theory”, **Y. Ping**, D. Rocca and G. Galli*, *Chemical Society Reviews*, **42**, 2437, (2013).

6. “Synthesis, Photoelectrochemical Properties, and First Principle Study of n-type $CuW_{1-x}Mo_xO_4$ Electrodes Showing Enhanced Visible Light Absorption”, J. Hill, **Y. Ping**, G. Galli*, K. Choi*, *Energy & Environmental Science (Communication),* **6**, 2440, (2013).

5. “Optical Properties of Tungsten Oxide from First Principles”, **Y. Ping***, D. Rocca, G. Galli, *Physical Review B,* **87**, 165203, (2013).

4. “Ab-initio Calculations of Absorption Spectra of Semiconducting Nanowires within Many Body Perturbation Theory”, **Y. Ping***, D. Rocca, D. Lu and G. Galli, *Physical Review B,* **85**, 035316, (2012).

3. “Bethe-Salpeter Equation Without Empty Electronic States: Application to Bulk Systems”, D. Rocca*, **Y. Ping**, G. Galli, *Physical Review B,* **85**, 045116, (2012).

2. “Thermally Stable N_2-intercalated WO_3 Photoanodes for Water Oxidation”, Q. Mi, **Y. Ping**, Y. Li, B. Brunschwig, G. Galli*, H. Gray* and N. Lewis*, *Journal of the American Chemical Society*, **134**, 18318, (2012). (Highlighted in the feature article of CCI Solar)

1. “Tungsten Oxide Clathrates for Water Oxidations: A First Principle Study”, **Y. Ping***, Y. Li, F. Gygi, G. Galli, *Chemistry of Materials*, **24**, 4252, (2012).

***Corresponding authors

Professional Services

Conference symposium organizer:

APS March Meeting focus topic on “First-principles modeling of excited-state phenomena in materials” (2019-2022)

ACS Spring National Meeting symposium topic on "Simulations of Materials and Processes for Energy Applications" (2019), "Frontier of Theory and Computation for Materials and Processes in Energy Applications" (2021)

Invited Talks and lectures:

CCI Solar Center at Caltech (2013), SUNCAT, SLAC National Accelerator Laboratory (2013), Molecular Foundry, LBNL (2013), American Physics Society March meeting (2014), Materials Science & Engineering, Darmstadt, Germany (2014), UC Santa Cruz (2016), UC Merced (2016), American Chemical Society Spring meeting (2017, 2019), International Conference on Chemical Bonding (2018), Molecular Foundry User Meeting (2018), CCI Solar Fuels Capstone Meeting (2018), International Conference on Defects in Semiconductors (2019), West Coast Theory Symposium (2019), GO2020(graphene online conference) (2020), Princeton University (2020), Yale University (2020), Washington University in St. Louis(2020), UC Santa Barbara (2020), UIUC (2020), USC (2021), RPI(2021), UT Austin (2021), UCLA(2021), Stanford (2021), Cal state-Long Beach (2021), MRS Spring meeting (2021), ECS meeting (2021), APS March meeting (2021), ACS Spring meeting (2021), CHOISE-EFRC (2021), Institut Català de Nanociència i Nanotecnologia (ICN2), Spain (2021), MRS Spring meeting (2022), MRS Fall meeting (2022),

Defects in Solids for Quantum Technologies at Sweden (2022), ACTC meeting (2022), ACS Fall meeting (2022)

Reviewer for peer-reviewed journals:
Nature Physics, Nature Computational Science, Nature Materials, Nature Communications, Physical Review Letters, Nature Energy, Joule, Nature Catalysis, Advanced Materials, Advanced Functional Materials, Advanced Optical Materials, Nano Letters, ACS Nano, NPJ Computational Materials, Physical Review B/E/Materials, Journal of Physics: Condensed Matter, Journal of Applied Physics, Journal of the American Chemical Society, the Journal of Physical Chemistry Letters, ACS Energy Letters, Chemistry of Materials, Nanoscale, Journal of Materials Chemistry A/C, ACS Applied Materials & Interfaces, Journal of Physical Chemistry, Journal of Chemical Physics, RSC Advances, Physical Chemistry Chemical Physics, ACS catalysis, Angewandte Chemie, Nano Research, 2D Materials

Reviewer for grant applications:
DOE (BES, CAREER)
NSF (DMR/CMMT, CHE/CTMC, CHE/Catalysis, CAREER)
DOD-AFSOR
ACS-Petroleum Fund

Invited Talks and Seminars

43. “First-principles many-body theory and quantum dynamics for materials in quantum information science”, ACS, Chicago, 2022.

42. “Ab-initio Spin Dynamics in Solids”, Rising Talent invited talk, ACTC, Lake Tahoe, 2022.

41. “Photophysics of Quantum Defects in Two-Dimensional Materials from First-Principles”, Defects in solids for quantum technologies, Sweden, 2022.

40. “Photophysics of Quantum Defects in Two-Dimensional Materials from First-Principles”, MRS Spring Meeting, 2022.

39. “First-Principles Many-Body Theory and Quantum Dynamics for Materials in Quantum Information Science”, Caltech, MRL seminar, 2022.

38. “Effect of Polaron Formation on Optical and Carrier Transport Properties of Transition Metal Oxides as Photoelectrodes”, AdvMatSyn22, NanoGe conference, 2022.

37. “First-Principles Materials Prediction: from Sustainability to the Quantum Information Age”, Institut Català de Nanociència i Nanotecnologia (ICN2), Barcelona, Spain, 2021.

36. “Ab initio ultrafast spin dynamics for solids”, CHOISE-EFRC, online, 2021.

35. “Photo-physics of Quantum Defects and Spin Dynamics from First-Principles Calculations”, Molecular Foundry, 2021

34. “Recombination and Spin Dynamics of Quantum Defects in Two Dimensions”, Brookhaven National Laboratory, 2021

33. “Ab initio ultrafast spin dynamics for solids”, MRS Spring meeting, 2021

32. “Ab initio ultrafast spin dynamics for solids”, ACS Spring meeting, (Invited talk by ACS COMP for open-eye outstanding junior faculty award), 2021.

31. “Quantum defects and recombination in two-dimensional materials”, APS March meeting, 2021.

30. “First-principles materials prediction: from sustainability to the quantum information age”, Stanford University, 2021.

29. “First-principles materials prediction: from sustainability to the quantum information age”, UT Austin, 2021.

28. “First-principles materials prediction: from sustainability to quantum information science”, RPI, 2021.

27. “First-principles materials prediction: from sustainability to quantum information science”, USC, 2021.

26. “First principles many-body theory and quantum dynamics for materials prediction”, UC Los Angeles, 2020.

25. “Spin dynamics and exciton recombination for materials in quantum information science”, Yale University, 2020.

24. “Spin dynamics and exciton recombination in quantum materials from first-principles”, University of Illinois Urbana-Champaign, 2020.

23. “Spin and exciton dynamics in quantum materials from first-principles”, UC Santa Barbara, 2020.

22. “Spin and exciton dynamics in two-dimensional materials from first-principles”, Washington University in St. Louis, 2020.

21. “Spin and exciton dynamics in quantum materials from first-principles”, Princeton University, 2020.

20. “Spin-phonon relaxation from a first-principles density matrix approach”, Graphene and 2DM Online conference, 2020.

19. “Charge and spin dynamics for defects in 2D materials for quantum information”, International Conference for Defects in Semiconductors (ICDS30), 2019.

18. “Charge and spin dynamics for defects in 2D materials from first-principles”, Peking University, 2019.

17. “Excited state dynamics of charged defects in two-dimensional materials from many body perturbation theory”, Northern California Theoretical Chemistry Meeting 2019 (UC Berkeley).

16. “Effects of defects on electron polaron formation and transport in transition metal oxides”, invited speaker, American Chemical Society Spring meeting 2019.

15. “Design Defects in Two-dimensional Materials for Quantum Information from First-principles”, University of California-Santa Cruz, Physics Colloquium, 2019.

14. “First-principles Study of Charged Defects**:** from single photon-emission to polaronic conduction”, University of California-Merced, 2019.

13. “Defects in Complex Materials for Energy Conversion and Quantum Information Applications”, San Francisco State University, 2018.

12. “Boost Small Polaron Conduction in Transition Metal Oxides by Atomic Doping”, Molecular Foundry User Meeting, 2018.

11. “Charged Defects in Two-dimensional Materials from Many Body Perturbation Theory”, International Conference on Chemical Bonding, Hawaii, 2018.

10. “Boost Polaronic Transport in Transition Metal Oxides by Atomic Doping from First-principles Calculations”, CCI Solar Fuels Capstone Meeting, Ventura, 2018.

9. “Boost Small Polaron Transport in Metal Oxides by Atomic Doping”, the 3rd Molecules and Materials for Artificial Photosynthesis, Cancun, Mexico, 2018.

8. “Light Absorbers, Interfaces and Catalysis for Solar-to-fuel conversion: First-Principles Calculations”, invited speaker, American Chemical Society Spring meeting 2017.

7. “Computational Materials Science for Solar Energy Conversion”, Condense Matter Seminar, University of California-Santa Cruz, 2016.

6. “Light Absorbers, Interfaces and Catalysts for Solar-to-fuel Conversion: First Principles Calculations”, University of California-Merced, 2016.

5. “Harvesting the Energy from the Sun: Insights from Atomistic and ab Initio Materials Modeling”, **Keynote lecture**, MSE 2014, Darmstadt, Germany, 2014.

4. “Light Absorbers for Photoelectrochemical Energy Conversion: First Principles Calculations”, invited speaker, American Physics Society March meeting, Denver, 2014.

3. “First Principles Calculations of the Electronic Properties of Light Absorber and Aqueous Interfaces”, All Hands meeting, JCAP, 2014.

2. “Electronic Excitations in Light Absorbers for Photoelectrochemical Energy Conversion from First-Principles Calculations”, SUNCAT, SLAC National Accelerator Laboratory; Molecular Foundry, Lawrence Berkeley National Laboratory; Materials and Process Simulation Center, Caltech, 2013.

1. “First Principles Calculations of Electronic Excitation Processes in Light Absorbers” CCI Solar center annual meeting, Caltech, 2013.