Dr. Yuan Ping

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

Developing theoretical and computational methods such as first-principles many-body theory and open quantum dynamics based on density-matrix formalism, to understand and predict materials' properties including optoelectronic, quasiparticle (e.g. excitons, polarons, magnons) dynamics and transport properties in solid-state systems, quantum defects, and heterogenous interfaces, for low-power electronics, quantum information science, and energy conversion applications. Current interests include:

- Electronic excitation and spectroscopy from many-body perturbation theory
- First-principles open quantum dynamics, with quantum scatterings of electron-electron and electron-phonon interactions, for spin, electron, magnon, and exciton dynamics.
- Quantum defects as spin qubits' optical readout and decoherence from first-principles
- Spin-optronics, chiral-optics, and nonlinear optics properties of solids

Appointments

July 2023-	Associate Professor, Materials Science and Engineering, University of Wisconsin, Madison
July 2023-	Adjunct Professor, Department of Physics, University of California, Santa Cruz
July 2023-	Affiliated Professor, Department of Physics and Department of Chemistry, University of Wisconsin, Madison
July 2022- July 2023	Associate Professor, Department of Chemistry and Biochemistry, University of California, Santa Cruz
July 2016-July 2022	Assistant Professor, Department of Chemistry and Biochemistry, University of California, Santa Cruz
July 2017- July 2023	Affiliated Professor, Department of Physics, University of California, Santa Cruz

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)
- Outstanding Student Scholarship (2003–2006)

Grants

Grants as single PI or lead PI:

- DOE BES Computational Chemical Science (DOE-CCS center, ADEPTs) Award, lead PI (2022-2026), $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, (2021-2025), $450,000, "First-principles Spin Relaxation in Two-Dimensional Materials: Proximity, Twisting and Doping Effects"

- Alfred Sloan Research Fellowship (2022-2026), $75,000, "First-Principles Theory for Materials in Quantum Information Science"

- NSF, Condensed Matter and Materials Theory, lead PI, Grant No. DMR-1956015 (2020-2024), $497,627 (Ping's share 266K), "CDS&E: Ab Initio Ultrafast Dynamics of Spin, Valley and Charge in Quantum Materials"

- 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:

- NSF, Macromolec/Supramolec/Nano, co-PI, Grant No. CHE-2505880, (2025-2028), $532,240 (Ping: $200,000), "Probing Ultrafast Carrier Spin Dynamics in Pb-free Metal Halide Double Perovskites"

- AFOSR CFIRE, co-PI, (2023-2026), Ping's share $750.001, "Unveiling and Controlling Quantum Point Defects in Oxides"

- DOE BES Computational Materials Science, co-PI, (2023-2026), Ping's share $600,000, "Center for non-Perturbative Studies of Functional Materials under Non-equilibrium Conditions" (DOE-CMS center, NENPQ, thrust lead)

- NSF MRSEC at UW-Madison, co-PI, (2023-2029), Ping's share $501,945

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

- Gordon and Betty Moore Foundation, co-PI, (2022-2027), $1.25M in total, "On-demand characterization of quantum defects in two-dimensional materials"

- 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 (2019-2023), $449,886 (Ping: $150,000), "Understanding and Enhancing Electronic Coupling Between Metal Halide Perovskites Quantum Dots through Surface Molecular Engineering"

Students and Postdocs Mentored

UW-Madison postdocs and scientists:
Gabriele Riva (postdoc, 2024 -)
Wuzhang Fang (postdoc, 2023 -)
Junting Yu (postdoc, 2024 -)
Mayank Gupta (postdoc, 2024 -)
Jacopo Simoni (scientist I, 2024 -)

UCSC postdocs:
Rafi Ullah (postdoc, 2023)
Sumit Naskar (postdoc, 2023)
Junqing Xu (postdoc, 2019-2023)
Hiroyuki Takenaka (postdoc, 2020-2022)
Feng Wu (postdoc, 2016-2019)

UW-Madison graduate student:
Shijie Fang (graduation student in Physics, 2025-)
Keynesh Dongol (graduate student in MSE, 2025-)
Shihao Tu (graduate student in MSE, 2024-)
Dorong Wu (graduate student in Chemistry, 2024-)
Erik Alfredo Perez (graduate student in MSE, 2023-)
Andrew Grieder (graduate student in MSE, 2023-; UCSC in chemistry 2021-2023)
Shiming Zhang (graduate student in MSE, 2023-; UCSC in physics 2020-2023)
Chunhao Guo (graduate student in MSE, 2023-2025(graduated); UCSC in chemistry 2018-2023)

UCSC graduate student:
Kejun Li (graduate student in physics, 2019-2024, graduated)

Tyler Smart (graduate student in physics, 2016-2021, graduated)
Zachary Sanders-Bellis (undergraduate, 2018-2020)
Remi Leano (undergraduate, 2018-2019)
Anikeya Aditya (undergraduate, 2018-2019)

Classroom Teaching

UW-Madison (2024-)
Molecular Modeling of Materials (MSE 760) (graduate level, 2024 fall)

UW-Madison (2023-)
Introduction to Computational Materials Science (MSE 460) (undergraduate level, 2023 spring)

UCSC (2017-2022)
Quantum Mechanics (Graduate level, 2017 spring – 2022 spring)

Quantum Mechanics and Basic Spectroscopy (Undergraduate level, 2017 fall -2022 fall)

Publications

Google scholar: https://scholar.google.com/citations?user=w8iecRcAAAAJ&hl=en
Citation: 6717, h-index 44

Under Review:

96. "Photogalvanic currents from first-principles real-time density-matrix dynamics", **Junting Yu, Andrew Grieder, Jacopo Simoni,** Ravishankar Sundararaman, Aris Alexandradinata**, Yuan Ping**, preprint, (2026), https://arxiv.org/abs/2601.01059

95. "Two-dimensional helical superconductivity and gapless superconducting edge modes in the 1T′-WS2/2H-WS2 heterophase bilayer", Xuance Jiang, Jennifer Cano, **Yuan Ping,** Yafis Barlas, Deyu Lu, submitted, (2025), https://arxiv.org/abs/2512.10157

94."The role of orbital polarization and spin-dependent electron-phonon scatterings in chiral-induced spin selectivity**", Mayank Gupta, Andrew Grieder,** Mayada Fadel, **Jacopo Simoni, Junting Yu,** Ravishankar Sundararaman*, and **Yuan Ping*,** submitted, (2025), https://arxiv.org/abs/2508.03886

93. "Spatio-temporal spin transport from first principles**",** Mayada Fadel, Joshua Quinton, Mani Chandra, **Mayank Gupta, Yuan Ping∗,** and Ravishankar Sundararaman*, submitted, (2025) https://www.arxiv.org/pdf/2505.07745

92. "Deep Spin Defects in Zinc Oxide for High-Fidelity Single-Shot Readout", **Shimin Zhang**,Taejoon Park, **Erik Perez, Kejun Li,** Xingyi Wang, Yanyong Wang, Jorge D Vega Bazantes, Ruiqi Zhang, Jianwei Sun, Kai-Mei C. Fu, Hosung Seo, and **Yuan Ping*,** in revision in Physical Review X Quantum, 2025. https://arxiv.org/abs/2502.00551

91. "Optical control of spin-splitting in an altermagnet", Sangeeta Rajpurohit, Revsen Karaalp, **Yuan Ping**, Liang Z Tan, Tadashi Ogitsu, Peter E Blöchl, under review, 2024.

Published/Accepted:

90. “First-principles open quantum dynamics for solids based on density-matrix formalism”, **Jacopo Simoni, Gabriele Riva, Yuan Ping***, invited perspective, Journal of Chemical Physics, 163, 170901 (2025).

89. **“**Spin non-Collinear Real-Time Time-Dependent Density-Functional Theory and Implementation in the Modern GPU-Accelerated INQ code**“,** Jacopo Simoni*, Xavier Andrade**, Wuzhang Fang, Andrew C. Grieder,** Alfredo A. Correa, Tadashi Ogitsu, and **Yuan Ping**, *APL Computational Physics*, https://arxiv.org/abs/2506.21908, (2025). **Selected as “Editor’s pick”.**

88. “Phonon-Assisted Radiative Lifetimes and Exciton Dynamics from First Principles”, **Chunhao Guo, Gabriele Riva, Junqing Xu, Jacopo Simoni, Yuan Ping**, *Physical Review B (Letters),* 112, L161111, (2025).

87. “Carrier Localization and Two-Dimensional Polarization Domain in Halide Perovskites”, **Andrew Grieder**, Marcos Calegari Andrade, **Hiroyuki Takenaka**, Tadashi Ogitsu, Liang Z. Tan, and **Yuan Ping***, *Physical Review Letters*, **135**, 136301, (2025). UW-Madison News

86. “Relation of Continuous Chirality Measure to Spin and Orbital Polarization, and Chiroptical Properties in Solids”, **Andrew Grieder, Shihao Tu, Yuan Ping***, *Advanced Optical Materials,* 13, e01190, (2025), https://doi.org/10.1002/adom.202501190

85. “Single nuclear spin detection and control in a van der Waals material”, Xingyu Gao, Sumukh Vaidya, **Kejun Li,** Saakshi Dikshit, **Shimin Zhang,** Peng Ju, Kunhong Shen, Yuanbin Jin, **Yuan Ping,** and Tongcang Li, *Nature,* 643*,* 943, (2025).

84. “Unconventional Superlattice Ordering in Intercalated Transition Metal Dichalcogenide V1/3NbS2.” Shannon Fender, Noah Schnitzer, and **Wuzhang, Fang**, Lopa Bhatt, Dingbin Huang, Amani Malik, Oscar Gonzalez, Veronika Sunko, Lilia Xie, David Muller, Joseph Orenstein, **Yuan Ping**, Berit Goodge, Kwabena Bediako. 2025. *Journal of the American Chemical Society* 147 (36): 32315–20.

83. “Exceeding the Critical Dopant Concentration Level: Substitution vs Oxide Precipitation in Fe2O3.” Mayford, Kiley, Samuel McNair, Mingpeng Chen, Bin Yao, **Andrew Grieder**, Samuel Eisenberg, Yat Li, **Yuan Ping,** and Frank Bridges. 2025. *Physical Review Materials* 9 (9). https://doi.org/10.1103/ryyl-vm3c.

82. “Anomalous Hall effect from inter-superlattice scattering in a noncollinear antiferromagnet”, LS Xie, SS Fender, C Mollazadeh, **W Fang,** MD Frontzek, S Husremović, Kejun Li, Isaac M Craig, Berit H Goodge, Matthew P Erodici, Oscar Gonzalez, Jonathan P Denlinger, **Yuan Ping**, D Kwabena Bediako, *Nature Communication*, in press, arXiv preprint arXiv:2411.08381 (2025).

81. “A cation-exchange approach to tunable magnetic intercalation superlattices”, Jingxuan Zhou, Jingyuan Zhou, Zhong Wan, Qi Qian, Huaying Ren, Xingxu Yan, Boxuan Zhou, Ao Zhang, Xiaoqing Pan, **Wuzhang Fang, Yuan Ping**, Zdenek Sofer, Yu Huang & Xiangfeng Duan, *Nature,* 643, 683, (2025). https://doi.org/10.1038/s41586-025-09147-z

80. “Efficient method for calculating magnon-phonon coupling from first principles“, **Wuzhang Fang, Jacopo Simoni, Yuan Ping*,** *Physical Review B*, 111, 104431, (2025).

79. “Magnetic-field dependence of spin-phonon relaxation and dephasing due to g-factor fluctuations from first principles”, J. Quinton, M. Fadel, **J. Xu,** A. Habib, M. Chandra, **Y. Ping*,** R. Sundararaman*, *Physical Review B*, 111, 115113, (2025).

78. “Colossal terahertz emission with ultrafast tunability based on van der Waals ferroelectric NbOI“, S. Subedi, W. Liu**, W. Fang,** C. Fox, Z. Zhai, F. Fei, **Y. Ping,** B. Lv, J. Xiao, *Advanced Optical Materials*, 13, 2403471, (2025). DOI: 10.1002/adom.202403471

77. “Enhancing the photoexcited charge carrier spin relaxation lifetime in CsPbBr3 perovskite quantum dots by 208Pb isotope enrichment“, Vivien L. Cherrette, David Zeitz, Mariam Khvichia, Jason K. Cooper, **Yuan Ping,** and Jin Z. Zhang, *The Journal of Physical Chemistry Letters,* 16, 3336, (2025).

76. “Proximity-Effect-Induced Remote Chirality Transfer in Hybrid Metal Halide Semiconductors“,Md Azimul Haque, **Andrew Grieder**, Steven P. Harvey, Roman Brunecky, Jiselle Y. Ye, Bennett Addison, Junxiang Zhang, Yifan Dong, Yi Xie, Matthew P. Hautzinger, Heshan Hewa Walpitage, Kai Zhu, Jeffrey L. Blackburn, Zeev Valy Vardeny, David B. Mitzi, Joseph J. Berry, Seth R. Marder, **Yuan Ping**, Matthew C. Beard, Joseph M. Luther*, *Nature Chemistry*, **17**, 29, (2024).

75. “Ultrafast Spin Relaxation of Charge Carriers in Strongly Quantum Confined Methylammonium Lead Bromide Perovskite Magic-Sized Clusters**”,** Zeitz, David; Cherrette, Vivien; Creech, Sarah; Li, Yan; **Ping, Yuan**; Zhang, Jin, *the Journal of Physical Chemistry Letters,* **4**, 610, (2024).

74. “First-Principles Computational Methods for Quantum Defects in Two-Dimensional Materials: A perspective“, Hosung Seo, Viktor Ivády, **Yuan Ping,** *Applied Physics Letters,* **125**, 140501, (2024).

73. “Excited-State Dynamics and Optically Detected Magnetic Resonance of Solid-State Spin Defects from First Principles“, **Kejun Li,** Vsevolod D. Dergachev, Ilya D. Dergachev, **Shimin Zhang,** Sergey A. Varganov, and **Yuan Ping*,** *Phys. Rev. B*, **110**, 184302, (2024).

72. “Spin-mechanical coupling in 2D antiferromagnet CrSBr“, Fei, Fan; Mao, Yulu; **Fang, Wuzhang**; Liu, Wenhao; Rollins, Jack; Kondusamy, Aswin; Lv, Bing; **Ping, Yuan**; Wang, Ying; Xiao, Jun, *Nano Lett.* **24**, 10467, (2024).

71. “Spin Dynamics in Hybrid Halide Perovskites -Effect of Dynamical and Permanent Symmetry Breaking“, **K. Li, J. Xu,** U., R. Bodin, M. Gupta, C. Multunas, J. Simoni, R.Sundararaman, Z. V. Verdany, and **Y. Ping*,** *The Journal of Physical Chemistry Letters,* **15**, 12156, (2024).

70. “Atomic Doping to Enhance the p-type Behavior of BiFeO3 Photoelectrodes for Solar H2O2 Production“, Daye Seo, † Andrew Grieder,† Andjela Radmilovic,† Sophya F. Alamudun, Xin Yuan, **Yuan Ping*** and Kyoung-Shin Choi*, *Journal of Materials Chemistry A,* **12**, 20437, (2024).

69. “Challenges in Advancing Our Understanding of Atomic-like Quantum Systems: Theory and Experiment”, Adam Gali, André Schleife, Andreas J. Heinrich, Arne Laucht, Bruno Schuler, Chitraleema Chakraborty, Christopher P. Anderson, Corentin Déprez, Jeffrey McCallum, Lee C. Bassett, Mark Friesen, Michael E. Flatté, Peter Maurer, Susan N. Coppersmith, Tian Zhong, Vijaya Begum-Hudde & **Yuan Ping**, *MRS Bulletin*, 49, 256, 2024.

68.“How Spin Relaxes and Dephases in Bulk Halide Perovskites”**, Junqing Xu†, Kejun Li†,** Uyen N. Huynh, Jinsong Huang, Ravishankar Sundararaman*, Valy Vardeny*, and **Yuan Ping***, *Nature Communications*, 15, 188, (2024). Engineering News.

67. “Circular Dichroism of Crystals from First Principles**”**, Christian Multunas, **Andrew Grieder, Junqing Xu, Yuan Ping*,** Ravishankar Sundararaman*, *Physical Review Materials*, 7, 123801, (2023)

66. “Ab-initio Predictions of Spin Relaxation, Dephasing and Diffusion in Solids**”**, **Junqing Xu** and **Yuan Ping*,** *Journal of Chemical Theory and Computation*, 20, 492, (2023), invited review.

65. “Effect of Environmental Screening and Strain on Optoelectronic Properties of Two-Dimensional Quantum Defects”**, Shimin Zhang, Kejun Li, Chunhao Guo**, and **Yuan Ping*,** *2D Materials*, **10**, 035036, (2023), preprint: http://arxiv.org/abs/2304.05612

64. “Comparative Electronic Structures of the Chiral Helimagnets $Cr_{1/3}NbS_2$ and $Cr_{1/3}TaS_2$**”** Xie, Lilia; Gonzalez, Oscar; **Li, Kejun;** Michiardi, Matteo; Gorovikov, Sergey; Ryu, Sae Hee; Fender, Shannon; Zonno, Marta; Jo, Na Hyun; Zhdanovich, Sergey; Jozwiak, Chris; Bostwick, Aaron ; Husremovic, Samra; Erodici, Matthew; Mollazadeh, Cameron; Damascelli, Andrea; Rotenberg, Eli; **Ping, Yuan**; Bediako, D., *Chemistry of Materials*, 35, 7239, (2023).

*Corresponding authors; **highlighted authors:** group members

Before UW-Madison (2016-2023):

63. “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*, *Advanced Materials*, **35**, 2206585, (2023). Underline authors are group members.

62. “Substrate effects on spin relaxation in two-dimensional Dirac materials with strong spin-orbit coupling”, Junqing Xu* and **Yuan Ping***, *npj Computational Materials*, **9**, 47, (2023) preprint: https://arxiv.org/abs/2206.00784

61. “Spin-defect qubits in two-dimensional transition metal dichalcogenides operating at telecom wavelengths”, Yeonghun Lee, Yaoqiao Hu, Xiuyao Lang, Dongwook Kim, Kejun Li, **Yuan Ping,** Kai-Mei C. Fu & Kyeongjae Cho*, *Nature Communications,* **13**, 7501, (2022).

60. “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*,** *Nanoscale*, **15**, 1619, (2022), Emerging Investigator Issue.

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*, **18**, 357, (2023). Underline authors are group members.

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,* **21**, 1024, (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).

Before UCSC: (Before 2016)

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 lead organizer:

- Telluride School for Theoretical Chemistry, co-chair, 2027.
- Electronic Structure Workshop lead organizer, 2026.
- Gorden Research Conference: Defects in Semiconductors, co-chair, 2026.

- MRS Spring Meeting Symposium QT06: Defects in Solid-State Materials for Quantum Technologies (2025)
- APS March Meeting focus session on “Theory for non-equilibrium Quantum Physics in Materials” (2025)
- APS March Meeting focus session on “First-principles modeling of excited-state phenomena in materials” (2019-2023)
- ACS Spring National Meeting symposium topic on "Frontier of Theory and Computation for Materials and Processes in Energy Applications" (2021)
- ACS Spring National Meeting symposium topic on "Simulations of Materials and Processes for Energy Applications" (2019)

Reviewer for peer-reviewed journals:
Nature, Nature Physics, Nature Materials, Nature Computational Science, Nature Communications, Nature Chemistry, Physical Review Letters, Nature Energy, Joule, Nature Catalysis, Science Advances, Advanced Materials, Advanced Functional Materials, Advanced Optical Materials, Nano Letters, Journal of the American Chemical Society, ACS Nano, NPJ Computational Materials, Physical Review B/E/Materials, Journal of Physics: Condensed Matter, Journal of Applied Physics, 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, QIS, CAREER)
NSF (DMR/CMMT, CHE/CTMC, CHE/Catalysis, CAREER)
DOD-AFSOR
ACS-Petroleum Fund

Invited Talks and Seminars

81. Invited Talk, ACS Spring meeting, 2026.

80. Invited Talk, GRC Computational Materials Science 2026.

79. Invited Seminar, Argonne National Laboratory, 2026.

78. Invited Talk, UCB Total Energy Mini Workshop, UCBerkeley 2026.

77. Invited Seminar in Cambridge University, December 2025.

76. CECAM Flagship Workshop “Recent advances in first-principles modeling of electron-phonon interactions”, EPFL, Lausanne, 2025.

75. Invited lectures, 2025 Telluride school in theoretical chemistry, 2025.

74. TSRC workshop, nonequilibrium phenomena, nonadiabatic dynamics and spectroscopy, 2025.

73. Psi-k 2025 Conference invited talk, EPFL, 2025.

72. Invited Seminar, Brookhaven National Laboratory, 2025.

71. “First-Principles Open Quantum Dynamics for Solids based on a Density-Matrix Formalism”, 55th Midwest Theoretical Chemistry Conference (MWTCC55), 2025.

70. DOE Workshop on spin induced selectivity: Spin-Charge-light conversion (NREL), 2025.

69. “Spin-optotronic Properties of Solids from Ab-initio Density-Matrix Dynamics”, Princeton Center for Theoretical Science workshop, 2025.

68. “Continuous Chirality measure on spin and orbital polarization, and optical activity in solids”, MRS Spring, 2025.

67. “Spin Relaxation and Optronics Properties of Solids from Ab-initio Density-Matrix Dynamics”, APS March meeting, 2025.

66. “Spin-optotronic Properties of Solids from Ab-initio Density-Matrix Dynamics”, MRS Fall 2024.

65. “First-Principles Many-Body Theory and Quantum Dynamics for Materials in Quantum Information Science”, GRC conference on Computational Materials Science and Engineering, 2024.

64. “Excited-State Dynamics and Optically Detected Magnetic Resonance of Solid-State Spin Defects from First Principles”, GRC conference on Defects in Semiconductors, 2024.

63. “Spin-optotronic properties from ab-initio density-matrix dynamics in semiconductors” LLNL Summer school invited talk, 2024.

62. “Ab-initio Quantum Dynamics for Spin Relaxation and Photogalvanic Effects in Perovskites”, DOE EFRC center mid-term review, 2024.

61. “First-principles Theory for Excited-State Kinetics and Optical Readout of Quantum Defects”, Physics Colloquium, Purdue University, 2024.

60. “Spin-optotronic properties from ab-initio density-matrix dynamics in solids”, CISS online meeting, 2024.

59. “First-principles Theory for Excited-State Kinetics and Optical Readout of Quantum Defects”, Physics Colloquium, University of North Texas, 2024.

58. “First-Principles Many-Body Theory and Quantum Dynamics for Materials in Quantum Information Science”, Physics Colloquium, Tulane University, 2023.

57. “First-Principles Many-Body Theory and Quantum Dynamics for Materials in Quantum Information Science”, Physics Colloquium, Washington University at Saint Louis, 2023.

56. “First-Principles Many-Body Theory and Quantum Dynamics for Solids”, Condensed Matter Seminar, Department of Physics, University of Wisconsin-Madison, 2023.

55. “Excited-State Dynamics of Spin Defects from First-Principles”, Balleroy Workshop, Chateau, France, invited talk, 2023.

54. “Ab-initio Open Quantum Dynamics for Spin and Electron Relaxation in Solids”, invited talk at EMP2023 Conference, NUSU, 2023.

53. “Spin Relaxation, Dephasing, and Diffusion in Solids from ab-initio Density-Matrix Dynamics”, Electronic Structure Workshop, UC Merced, 2023.

52. “First-Principles Many-Body Theory and Quantum Dynamics for Solids”, Center for Computational Chemistry at NYU Shanghai, online seminar, 2023.

51. “Ab-initio Open Quantum Dynamics for Spin and Electron Relaxation in Solids”, AFOSR annual review, invited talk 2023.

50. “Spin Relaxation and Dephasing in Solids from ab-initio Density-Matrix Dynamics”, Kavli ENSI workshop on spintronics, UC Berkeley 2023.

49. “Spin Relaxation and Dephasing in Solids from ab-initio Density-Matrix Dynamics”, APS March meeting, Las Vegas, 2023.

48. “Ab-initio Open Quantum Dynamics for Spin and Electron Relaxation in Solids”, 4th Berkeley Excited States Conference (BESC2023).

47. “Ab-initio Open Quantum Dynamics for Spin and Electron Relaxation in Solids”, 62nd Sanibel Symposium, Florida, 2023.

46. “First-Principles Many-Body Theory and Quantum Dynamics for Materials in Quantum Information Science”, Materials Science and Engineering, University of Illinois Urbana-Champaign, 2022.

45. “Effect of Polaron Formation on Optical and Carrier Transport Properties of Transition Metal Oxides As Photoelectrodes from First-Principles Calculations”, MRS Fall meeting (virtual), 2022.

44. “Effect of Polaron Formation on Optical and Carrier Transport Properties of Transition Metal Oxides As Photoelectrodes from First-Principles Calculations”, 242th ECS meeting in Atlanta, 2022.

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.