Hsin-Yu Ko, Ph.D.

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Education

Department of Chemistry, **Princeton University**, Princeton, NJ, USA

- Ph.D./M.A in Theoretical Chemistry with Professor Roberto Car **09/2012 – 01/2019**

  Thesis: *First-Principles Study on the Structural and Thermal Properties of Molecular Crystals and Liquids*

  Research: (*i*) Enabling an accurate and reliable prediction of the structural and thermal properties of dispersion-bound molecular crystals. (*ii*) Developing and implementing an efficient and scalable framework that enables large-scale *ab initio* molecular dynamics (AIMD) in condensed-phase environments using meta-generalized-gradient approximation (meta-GGA) and hybrid density functional theory (DFT). (*iii*) Developing local structure based metrics that provide a sensitive gauge to condensed-phase environments and a viable order parameter for studying crystallization. (*iv*) Applying the developments above to the study of liquid water, ice, metal-oxide surfaces, and molecular crystals.

  Teaching: General Chemistry Labs (four semesters).

Department of Chemistry, **National Taiwan University**, Taipei, Taiwan

- B.S. in Chemistry (*summa cum laude*) with Professor Bih-Yaw Jin **09/2006 – 06/2010**

  Thesis: *Theoretical Studies on the Optical Properties of Carbon Nanostructures*

  Research: Developed and applied semi-empirical quantum chemistry and free-electron methods with 2D spatial constraints to model the optical responses of carbon nanostructures.

Job Experience

Department of Chemistry and Chemical Biology, **Cornell University**, Ithaca, NY, USA

- Postdoctoral Research Associate with Professor Robert A. DiStasio Jr. **07/2019 – present**

  Research: (*i*) Developing efficient condensed-phase electronic structure algorithms for next-generation exascale supercomputing architectures. (*ii*) Constructing machine-learning-based representations for the interatomic interactions occurring for studying alkaline solutions. (*iii*) Modeling OH^- conductivity through anionic-exchange membranes in alkaline fuel cells.

Department of Chemistry, **Princeton University**, Princeton, NJ, USA

- Postdoctoral Research Associate with Professor Roberto Car **02/2019 – 06/2019**

  Research: (*i*) Enabling extended length- and time-scale of AIMD based simulation to study isotope effects in water via deep neural network. (*ii*) Applying AIMD to studying H-bond network in supercritical water.

Department of Chemistry, **National Taiwan University**, Taipei, Taiwan

- Research Assistant with Professor Bih-Yaw Jin **08/2011 – 07/2012**

  Research: Studied electromagnetic responses of metal-organic complexes using quantum mechanical tight-binding models.

  Teaching: Mathematical Techniques in Chemistry (one semester).

Professional Affiliations

- American Chemical Society (**ACS**)/**COMP division**; member number: **31522951**
- American Physical Society (APS)
- Materials Research Society (MRS)

Scientific Software

- Active Contributor / Developer

  Quantum ESPRESSO **2012 – present**

Honors and Awards

- NERSC Early Career Award for High Impact Scientific Achievement, NERSC **2021**
- Pickering Teaching Award, Princeton University **2016**
- Natural Sciences and Engineering Fellowship, Princeton University **2013**
- Studying Abroad Scholarship, Ministry of Education of Taiwan **2012**
- Research Poster Award, Chinese Chemical Society **2011**
- Phi Tau Phi Scholastic Honor Society, Taiwan **2010**
- Dean's Award, National Taiwan University **2010**
- Research Poster Award, National Taiwan University **2010**
- Dean's List (four times), National Taiwan University **2006 – 2010**

Metrics

Citations: 4099 h-index: 13 i10-index: 15 (Google Scholar; updated on 2021-12-07)

Publications

25. **H.-Y. Ko**, Z. M. Sparrow, M. F. C. Andrade, R. A. DiStasio Jr., *exx-β: Accurate and Efficient Order-N Framework for Hybrid DFT Based Ab Initio Molecular Dynamics of Heterogeneous Finite-Gap Condensed-Phase Systems*, (**in preparation**).
24. **H.-Y. Ko**, Z. M. Sparrow, R. A. DiStasio Jr., *SeA: Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based High-Throughput Calculations*, (**in preparation**).
23. Z. M. Sparrow, **H.-Y. Ko**, R. A. DiStasio Jr., *Enabling Linear Scaling Exact Exchange for Heterogeneous Systems*, (**in preparation**).
22. Y. Yang, Y.-T. Shao, X. Lu, Y. Yang, **H.-Y. Ko**, R. A. DiStasio Jr., F. J. DiSalvo, D. A. Muller, H. D. Abruña, *Elucidating Cathodic Corrosion Mechanisms with Operando Electrochemical Transmission Electron Microscopy*, (**in review**).
21. Y. Yang, . . . , **H.-Y. Ko**, . . . , *Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies*, Chem. Rev. (**in press**). Cover Article
20. **H.-Y. Ko**, B. Santra, and R. A. DiStasio Jr., *Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics II: Extensions to the Isobaric-Isoenthalpic and Isobaric-Isothermal Ensembles*, J. Chem. Theory Comput. **17**, 7789 (2021).
19. W. You, J. M. Ganley, B. G. Ernst, C. Peltier, **H.-Y. Ko**, R. A. DiStasio Jr., R. R. Knowles, and G. W. Coates, *Expeditious Synthesis of Aromatic-Free Piperidinium-Functionalized Polyethylene as Alkaline Anion Exchange Membranes*, Chem. Sci. **12**, 3898 (2021). Chem. Sci. HOT Article
18. C. Andreani, G. Romanelli, A. Parmentier, R. Senesi, A. I. Kolesnikov, **H.-Y. Ko**, M. F. Calegari Andrade, and R. Car, *Hydrogen Dynamics in Supercritical Water Probed by Neutron Scattering and Computer Simulations*, J. Phys. Chem. Lett. **11**, 9461 (2020).
17. **H.-Y. Ko**, J. Jia, B. Santra, X. Wu, R. Car, and R. A. DiStasio Jr., *Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics I: Theory, Algorithm, and Performance*, J. Chem. Theory Comput. **16**, 3757 (2020).
16. F. Tang, X. Jiang, **H.-Y. Ko**, J. Xu, M. Topsakal, G. Hao, A. T. N'Diaye, P. A. Dowben, D. Lu, X. Xu, and X. Wu, *Probe Ferroelectricity by X-ray Absorption Spectroscopy in Molecular Crystal*, Phys. Rev. Materials **4**, 034401 (2020).
15. T. Suh, Y. Yang, P. Zhao, K. U. Lao, **H.-Y. Ko**, J. Wang, R. A. DiStasio Jr., and J. Engstrom, *Competitive Adsorption as a Route to Area-Selective Deposition*, ACS Appl. Mater. Interfaces **12**, 9989 (2020).
14. M. F. Calegari Andrade, **H.-Y. Ko**, L. Zhang, R. Car, and A. Selloni, *Free Energy of Proton Transfer at the Water - TiO_2 Interface from Ab Initio Deep Potential Molecular Dynamics*, Chem. Sci. **11**, 2335 (2020).
13. **H.-Y. Ko**, L. Zhang, B. Santra, H. Wang, W. E, R. A. DiStasio Jr., and R. Car, *Isotope Effects in Liquid Water via Deep Potential Molecular Dynamics*, Mol. Phys. **117**, 3269 (2019). Invited Article
12. J. Hoja, **H.-Y. Ko**, M. A. Neumann, R. Car, R. A. DiStasio Jr., and A. Tkatchenko, *Reliable and Practical Computational Prediction of Molecular Crystal Polymorphs*, Science Adv. **5**, eaau3338 (2019).

11. M. F. C. Andrade, **H.-Y. Ko**, R. Car, and A. Selloni, *Structure, Polarization, and Sum Frequency Generation Spectrum of Interfacial Water on Anatase TiO_2*, J. Phys. Chem. Lett. **9**, 6716 (2018).
10. B. Santra, **H.-Y. Ko**, Y. W. Yeh, F. Martelli, I. Kaganovich, Y. Raitses, and R. Car, *Root-Growth of Boron Nitride Nanotubes: Experiments and Ab Initio Simulations*, Nanoscale **10**, 22223 (2018). Back Cover Article
9. **H.-Y. Ko**, R. A. DiStasio Jr., B. Santra, and R. Car, *Thermal Expansion in Dispersion-Bound Molecular Crystals*, Phys. Rev. Materials **2**, 055603 (2018).
8. L. Zheng, M. Chen, Z. Sun, **H.-Y. Ko**, B. Santra, P. Dhuvad, and X. Wu, *Structural, Electronic, and Dynamical Properties of Liquid Water by Ab Initio Molecular Dynamics Based on SCAN Functional within the Canonical Ensemble*, J. Chem. Phys. **148**, 164505 (2018). EditorâĂŹs Pick
7. M. Chen, L. Zheng, B. Santra, **H.-Y. Ko**, R. A. DiStasio Jr., M. L. Klein, R. Car, and X. Wu, *Hydroxide Diffuses Slower than Hydronium in Water Because its Solvated Structure Inhibits Correlated Proton Transfer*, Nat. Chem. **10**, 413 (2018).
6. F. Martelli, **H.-Y. Ko**, E. C. Oguz, and R. Car, *Local-Order Metric for Condensed-Phase Environments*, Phys. Rev. B **97**, 064105 (2018).
5. F. Martelli, **H.-Y. Ko**, C. C. Borallo, and G. Franzese, *Structural Properties of Water Confined by Phospholipid Membranes*, Front. Phys. **13**, 136801 (2018).
4. P. Giannozzi, ..., **H.-Y. Ko**, ..., *Advanced Capabilities for Materials Modelling with Quantum ESPRESSO*, J. Phys.: Condens. Matter **29**, 465901 (2017).
3. M. Chen, **H.-Y. Ko**, R. C. Remsing, M. F. C. Andrade, B. Santra, Z. Sun, A. Selloni, R. Car, M. L. Klein, J. P. Perdew, and X Wu, *Ab Initio Theory and Modeling of Water*, Proc. Natl. Acad. Sci. USA **114**, 10846 (2017).
2. A. M. Reilly, ..., **H.-Y. Ko**, ..., *Report on the Sixth Blind Test of Organic Crystal Structure Prediction Methods*, Acta Crystallogr., Sect. B: Struct. Sci. **72**, 439 (2016).
1. Y. Shen, **H.-Y. Ko**, Q. Ai, S.-M. Peng, and B.-Y. Jin, *Molecular Split-Ring Resonators Based on Metal String Complexes*, J. Phys. Chem. C **118**, 3766 (2014).

Invited Presentations

4. "Towards an Accurate and Efficient Order-N HPC Framework for Large-Scale Condensed-Phase Hybrid Density Functional Theory", *Oral*, NERSC Seminar Series (2021).
3. "Quantum Espresso and GPU implementation of *Ab Initio* Molecular Dynamics (part II)", *Oral*, CSI Center Workshop (2019).
2. "Thermal Expansion in Dispersion-Bound Molecular Crystals", *Oral*, Cornell Theoretical Chemistry Division Journal Club (2019).
1. "Anharmonic Effects from Dispersion in Weakly Bound Molecular Crystals", *Poster*, Modeling Many-Body Interactions (MMBI15) Workshop (2015).

Contributed Presentations

17. "Enabling Linear Scaling Exact Exchange for Heterogeneous Systems", *Oral*, APS March Meeting (2021).
16. "Improving the Scalability of Condensed-Phase Hybrid Density Functional Theory: Computation, Communication, and Load Balancing", *Oral*, APS March Meeting (2020).
15. "Enabling Large-Scale *Isobaric-Isothermal* Hybrid Density Functional Theory Simulations in the Condensed Phase", *Oral*, APS March Meeting (2019).
14. "Thermal Expansion of Dispersion-Bound Molecular Crystals", *Poster*, Princeton Chemistry Retreat (2018).
13. "A Hybrid Version of the SCAN Functional Including Long-Range Dispersion Interactions", *Oral*, APS March Meeting (2017).
12. "A Hybrid Version of the van der Waals Inclusive SCAN Functional", *Poster*, SCAN Workshop (2017).
11. "The Role of Anharmonicity and Nuclear Quantum Effects in the Pyridine Molecular Crystal: An *Ab Initio* Molecular Dynamics Study", *Oral*, APS March Meeting (2016).
10. "Large-Scale Hybrid Density Functional Theory Calculations in the Condensed-Phase: *Ab Initio* Molecular Dynamics in the Isobaric-Isothermal Ensemble", *Poster*, APS March Meeting (2016).

9. "Large-Scale *Ab Initio* Isobaric-Isothermal Simulations Using Self-Consistent van der Waals Inclusive Density Functionals", *Poster*, PICSciE Workshop (2016).
8. "A General Purpose Massively Parallel *Ab Initio* Molecular Dynamics Implementation with a Linear Scaling Exact Exchange Algorithm", *Poster*, PICSciE Workshop (2015).
7. "*Ab Initio* and Classical Simulations of the Condensed Phase Using High-Performance Computing", *Poster*, ICTP Total Energy Meeting (2015).
6. "Large-Scale *Ab Initio* Isobaric-Isothermal Simulations Using Self-Consistent van der Waals Inclusive Density Functionals", *Poster*, SciDAC (DOE) Meeting (2015).
5. "Large-Scale *Ab Initio* Isobaric-Isothermal Simulations Using Self-Consistent van der Waals Inclusive Density Functionals", *Poster*, Princeton Chemistry Retreat (2015).
4. "Van der Waals Interactions in Pyridine and Pyridine-Like Molecular Crystals: An *Ab Initio* Molecular Dynamics Study", *Oral*, APS March Meeting (2014).
3. "All-In-One Scientific Research with SageTeX", *Oral*, PyCon Taiwan (2012).
2. "Simple Analytical Expressions for the Persistent Current and Anapole Moment of Carbon Nanotori in the Thin Tubular Limit", *Poster*, Annual Meeting of Chinese Chemical Society (2011).
1. "Theoretical Study of Quantum Particles Constrained on a $D_{n\mathrm{h}}$ Toroidal Surface–A Simple Free Electron Model for π-Electronic Structures of a Toroidal Carbon Nanotube", *Poster*, National Taiwan University (2010).

Mentoring and Outreach

- CSI Computational Chemical Science Center, Princeton University **2018**
  Serve as the BES Early Career Network (ECN) representative of the CSI center at Princeton to connect with other US Department of Energy (DOE) funded research centers.
- Princeton University **2016**
  Co-mentor for an undergraduate student participating in the Summer Undergraduate Research Program (Catalyzing Diversity in Chemistry Leadership).
- Princeton Association of Taiwanese Students (PATS) **2016**
  Volunteer web administrator.
- Princeton University **2014**
  Co-mentor for an undergraduate student participating in the Summer Undergraduate Research Program (Catalyzing Diversity in Chemistry Leadership).
- NYU Courant Institute of Mathematical Sciences **2014**
  Co-mentor for female high school student participating in The Girls' Science, Technology, Engineering, and Mathematics (GSTEM) summer research program.
- National Taiwan Science Education Center **2012**
  Volunteer lecturer on molecular models for elementary school students.
- Molecular Beading Exhibition, Taipei, Taiwan **2011**
  Volunteer organizer and demonstrator for the general public.
- National Taiwan University **2011**
  Volunteer lecturer on molecular structure theory for high school students.
- 2009 National Taiwan University Chemistry Camp **2009**
  Volunteer lecturer on chemical kinetics for high school students.

Professional Activities

- Organizer / Co-Organizer / Volunteer
  Quantum ESPRESSO and GPU Workshop, CSI Center, Princeton University **2019**
  Science Communication Webinar, DOE BES ECN **2019**
  ECN Meetup, APS March Meeting **2019**
  Morrel Cohen Symposium, Princeton University **2017**
  Chemistry Student-Invited Lecture Series (SILS), Princeton University **2017**
  Quasicrystal Conference, National Taiwan University **2012**
- Peer Review: J. Chem. Phys.; J. Phys.: Condens. Matter; Electron. Struct.

Professional Collaborators (Last 2 Years) Roberto Car (Princeton University), Mohan Chen (Temple University/Peking University), Robert A. DiStasio Jr. (Cornell University), Weinan E (Princeton University), Giancarlo Franzese (University of Barcelona), Michael L. Klein (Temple University), Fausto Martelli (IBM), John P. Perdew (Temple University), Biswajit Santra (Temple University), Annabella Selloni (Princeton University), Alexandre Tkatchenko (University of Luxembourg), Han Wang (Institute of Applied Physics and Computational Mathematics), and Xifan Wu (Temple University).

Grants and Computer Allocations

- ASCR Leadership Computing Challenge (ALCC) Award of 175 M CPU Hours **2015**
  Argonne National Laboratories and the U.S. Department of Energy (DOE)
  Project Name: *Anomalous Density Properties and Ion Solvation in Liquid Water: A Path-Integral Ab Initio Study*
  PI: Robert A. DiStasio Jr.
  Co-PIs: Biswajit Santra, Fausto Martelli, **Hsin-Yu Ko**, Xifan Wu, Michele Cerriotti, Annabella Selloni, and Roberto Car
- ASCR Leadership Computing Challenge (ALCC) Award of 350 M CPU Hours **2014**
  Argonne National Laboratories and the U.S. Department of Energy (DOE)
  Project Name: *Ion Solvation, Catalytic Interfaces, and Extreme Aqueous Environments: An Ab Initio Study of Liquid Water*
  PI: Robert A. DiStasio Jr.
  Co-PIs: David Limmer, Biswajit Santra, Fausto Martelli, **Hsin-Yu Ko**, Michele Cerriotti, Annabella Selloni, and Roberto Car