# DINGXIN FAN

**Postdoctoral Research Associate**

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## PROFESSIONAL PREPARATION

B.S. in Chemical Engineering, GPA:3.95/4.00
Departmental Honors, Graduated with Highest Distinction
**Purdue University**
2011 – 2015  West Lafayette, IN

Ph.D. in Chemical Engineering, GPA:3.96/4.00
**The University of Texas at Austin**
2015 – 2021  Austin, TX

Postdoc at Princeton Institute for the Science and Technology of Materials
**Princeton University**
2022 – Present  Princeton, NJ

## AWARDS

- Winner of PetroPhase2021 Best Student Poster Award, 2021
- APS-Division of Materials Physics Ovshinsky Student Travel Awards, 2021
- Dr. Robert Schechter Endowed Fellowship in ChE, 2020
- James R. and Merle Fair Endowed Graduate Fellowship in ChE, 2020
- Charles M. Simmons Endowed Presidential Fellowship in Engineering, 2017
- Cindy and Mike Zeglin Endowed Undergraduate Scholarship in ChE, 2015
- Dean's List & Semester Honors, Purdue University, 2011-2015

## PROJECTS

### First-principles studies of transition metal based catalysts

- Performed DFT calculations with a Hubbard *U* correction (DFT + *U*) to predict structures, magnetic structures and relative stability of metal (Mn, Fe, Co, Ni) oxides, hydroxides and oxyhydroxides. – *J. Phys. Chem. C* **119**, 32 (2015)
- Used previously established DFT + *U* method to elucidate the catalytically active phase for NiFe and CoFe layered double hydroxides for oxygen evolution reaction. – *Nat. Commun.*, **11**, 2522 (2020)

### Atomic force microscopy (AFM) simulation

- Simulated high-resolution AFM images of organic molecules with various functionalized probe tips (CO, $H_2$, $N_2$, Br and $CH_2O$) to understand contrast inversion phenomenon and image distortion using real-space DFT calculations. – *J. Vac. Sci. Technol. B* **35**, 04H102 (2018)
- Illustrated recent algorithmic developments to computing quantum forces that can produce accurate simulations of nc-AFM images for large and complex molecular species, and suggested new pathways to overcome current challenges in this rapidly evolving field. – *Phys. Rev. Mater.*, **3**, 110302 (2019)
- Discovered distinct topological characteristics associated with carbon-carbon triple bonds, and proposed a correlation to compute the amount of double bond character in a carbon-carbon bond based on the corresponding apparent bond length. – *Nano Lett.* **19**, 8, 5562-5567 (2019)
- Revealed the chemical and steric effects in AFM images of nonplanar organic molecules on metallic substrates, and proposed an approach to increase the visibility of certain functional groups. – *Phys. Rev. Mater.*, **00**, 003800 (2020)
- Calculated the required mechanical forces applied by the AFM probe to physically break a covalent chemical bond in a joint experimental-theoretical work. – *Nat. Commun.*, **12**, 5635 (2021)
- Proposed an algorithm to systematically identify heteroatoms (S,I and N) from C atoms using AFM. – *Small*, 2102977 (2021)

## LIFE PHILOSOPHY

*"There are three deaths. The first is when the body ceases to function. The second is when the body is consigned to the grave. The third is that moment, sometime in the future, when your name is spoken for the last time."*

## EXPERTISE

- Computational Physics/Chemistry
- Density Functional Theory
- Atomic Force Microscopy Simulation
- Numerical Methods
- Teaching

## PROGRAMMING

**Matlab**
**Fortran**
**Python**
**Bash**
**R**
**C**

## LANGUAGES

**Mandarin Chinese, Native**
**English**
**Japanese**

## MEMBERSHIPS

- American Physical Society (APS)
- American Chemical Society (ACS)
- American Institute of Chemical Engineer (AICHE)
- The Catalysis Club of Chicago (CCC)

## SKILLS

DFT Code: PARSEC | VASP | GPAW
Visualization: VMD | VESTA | Atomic Simulation Environment
Operating system: Windows | Linux
Software: Mathematica | LAMMPS | Microsoft Office | LaTeX | ChemDraw | JMP | Visual Studio Code | Aspen | Minitab | Photoshop | Illustrator

# PUBLICATIONS

**1.** Z. Zeng, M. Chan, Z. Zhao, J. Kubal, ***D. Fan*** and J. Greeley, "Towards First Principles-based Prediction of Highly Accurate Electrochemical Pourbaix Diagrams," *J. Phys. Chem. C* **119**, 32 (2015)

**2.** ***D. Fan***, "First-Principles Studies of Bulk and Surface Properties of Heterogeneous Catalysts and Electrocatalysts," Purdue University - Chemical Engineering Department Undergraduate Honors Thesis (2015)

**3.** ***D. Fan***, Y. Sakai and J. R. Chelikowsky, "Real-space Pseudopotential Calculations for Simulating Noncontact Atomic Force Microscopy Images*," *J. Vac. Sci. Technol. B* **35**, 04H102 (2018)
****Chosen to be the cover of the JVST B July/August 2018 issue; featured article; editor's pick; background graphics for the AVS 68 promotional materials***

**4.** ***D. Fan***, Y. Sakai and J. R. Chelikowsky, "Discrimination of Bond Order in Organic Molecules Using Noncontact Atomic Force Microscopy," *Nano Lett.* **19**, 8, 5562-5567 (2019)

**5.** J. R. Chelikowsky, ***D. Fan***, A. J. Lee and Y. Sakai, "Simulating Atomic Force Microscopy Images," *Phys. Rev. Mater.*, **3**, 110302 (2019) ****Highlighted prominently on* Phys. Rev. Mater. *Research Updates.***

**6.** ***D. Fan***, Y. Sakai and J. R. Chelikowsky, "Chemical and Steric Effects in Simulating Non-contact Atomic Force Microscopy Images of Organic Molecules on a Cu (111) Substrate," *Phys. Rev. Mater.*, **4**, 053802 (2020)

**7.** F. Dionigi, Z. Zeng, I. Sinev, T. Merzdorf, S. Deshpande, M. B. Lopez, S. Kunze, I. Zegkinoglou, H. Sarodnik, ***D. Fan***, A. Bergmann, J. Drnec, J. F. de Araujo, M. Gliech, D. Teschner, J. Greeley, B. R. Cuenya and P. Strasser, "In-situ Crystal Structure and Synergistic Reaction Mechanism for NiFe and CoFe Layered Double Hydroxide Catalysts in the Oxygen Evolution Reaction," *Nat. Commun.*, **11**, 2522 (2020) ****2020 Top 50 Chemistry and Materials Sciences Articles***

**8.** ***D. Fan****, P. Cheng*, A. Selloni, E. A. Carter, C. B. Arnold, D. C. Dankworth, S. P. Rucker, J. R. Chelikowsky, N. Yao and Y. Zhang, "Breaking a Dative Bond with Mechanical Forces." *Nat. Commun.*, **12**, 5635 (2021) ****Editors' Highlights, featured article in Inorganic and Physical Chemistry***

**9.** ***D. Fan*** and J. R. Chelikowsky, "Atomic Fingerprinting of Heteroatoms Using Noncontact Atomic Force Microscopy." *Small*, **17**, 2102977 (2021)

**10.** ***D. Fan***. "Seeing Molecules – Real-space Simulations of Noncontact Atomic Force Microscopy," Ph.D. Dissertation (2021)

**11.** ***D. Fan***, Y. Sakai, D. Meuer, J. R. Chelikowsky and F. J. Giessibl, "SPM Image Flickering on a Si(111) 7×7 Reconstructed Surface," *Phys. Rev. Lett.*, submitted (2021)

**12.** ***D. Fan****, P. Cheng*, J. R. Chelikowsky and N. Yao, "The Limit of Chemical Identification using Noncontact Atomic Force Microscopy," in preparation

**13.** ***D. Fan****, Y. Zhang*, L. Gross and J. R. Chelikowsky, "The Aromatic Pathways in Porphyrins of Different Charge States," in preparation

*: These authors contribute equally

# PRESENTATIONS

**1.** First Annual Purdue AIChE Undergraduate Research Poster Symposium, "CO, $NO_2^-$ and N adsorption on Pt and Cu surfaces." 2014

**2.** APS March Meeting, "Simulations of atomic force microscopy image 'flickering' on a doped Si (111) 7x7 surface using real-space pseudopotential calculations." 2018

**3.** APS March Meeting, "Using real space pseudopotentials to simulate non-contact atomic force microscopy images of organic molecules." 2019

**4.** APS March Meeting, "Discriminating functional groups, atomic species and molecular geometries in organic molecules using real-space simulations of non-contact atomic force microscopy." 2020

**5.** APS March Meeting, "Using real-space simulations of non-contact atomic force microscopy to distinguish functional groups, atomic species and molecular geometries in organic molecules." 2021

**6.** PetroPhase 2021, "Using real-space simulations of non-contact atomic force microscopy to distinguish functional groups, atomic species and molecular geometries in organic molecules." 2021 ****Best Student Poster Award***