Dong Zhou

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SUMMARY

Physicist and programmer, passionate about method development and innovation. 30+ papers with 2k+ citations, Erdös number ≤ 5, 1k+ stars on GitHub. Past experience includes crystal structure prediction, medical imaging, quantum computing, and spectro-microscopy.

SKILLS

Python, Go, C, Bash, AWS/GCloud
Computational physics/mathematics, Image processing, Machine learning

EXPERIENCE

- **Senior Developer I then II, Schrödinger Inc.**   2016-2024

  Main contributor to the crystal structure prediction product in the 0 to 1 stage (invented a divide-and-conquer optimization method for crystal packing search; speedup with analytical gradients for geometric operations, Cythonization, and two-stage convergence; workflow automation with GNU Make). Maintained atom mapping module (subgraph isomorphism) for free energy perturbation (FEP). Implemented atom mapping schemes for lambda dynamics, fragment linking, and linker enumeration FEP (Python). Implemented analysis library for molecular dynamics trajectories (Python, C++). Maintained scientific computing web services for FEP+ (aws/gcloud, Go, Python, PostgreSQL, gRPC, Docker, Polymer.js).

- **Postdoc in radiology, Weill Medical College of Cornell University**   2012–2016

  Invented a novel method (LBV) for background magnetic field removal using full multigrid solver. Solved ill-posed inverse problems using Bayesian inference such as magnetic susceptibility and susceptibility tensor imaging, magnetic quadrupole imaging, 3D phase unwrapping (Matlab, C/C++). Developed probes for transcranial magnetic stimulation both in simulation (COMSOL multiphysics) and on hardware (electronics, 3D printing).

- **Postdoc in physics, Yale University**   2011–2012

  Developed state preparation scheme using quantum bath engineering, and adiabatic phase based two-qubit CNOT gate scheme on circuit QED hardware (3D transmon). Simulated these schemes using Python package QuTip.

- **Research assistant, University of Wisconsin-Madison**   2007–2011

  Solved open quantum systems dynamics in the presence of classical stochastic noises both analytically and numerically (Matlab). Developed schemes for quantum gate, quantum control, and entanglement preparation for quantum dot systems. Developed algorithm for graph isomorphism problem using continuous-time quantum random walk. Performed experiments and data analyses for biological and geological samples such as nacre, pyrite, etc (machining, X-ray diffraction, X-ray absorption near edge spectroscopy and microscopy using synchrotron radiation @ SRC and LLNL). Implemented GUI program for spectra analysis (KaleidaGraph).

EDUCATION

- Ph.D in physics, University of Wisconsin-Madison (GPA 4.0, 71 credits)   2006–2011
- Graduate study in physics, University of Georgia-Athens (GPA 4.0, 49 credits)   2004–2006
- B.S. from Honored Mixed Class, Zhejiang University (GPA 3.8, 196 credits)   2000–2004

Honors and Awards

- International Society for Magnetic Resonance in Medicine (ISMRM) Merit Award, Magna Cum Laude, 2014
- International Student Academic Achievement Award, UW-Madison, 2011
- Ray and Anne Herb Award for Wisconsin Distinguished Graduate Fellowship, 2008
- Emanuel R. Piore Award for Highest Scorer on the Qualifier Exam, UW-Madison, 2007
- University Housing's Favorite Instructor Award for Fall 2006, UW-Madison, 2006
- Van Vleck Fellowship for Graduate Students in Physics, UW-Madison, 2006
- Honored Graduate of Zhejiang University, China, 2004
- Honorary Enrollment, Zhejiang University, China, 2000
- Tan Jiazhen (C. C. Tan) Scholarship for Outstanding High School Student in Biology, 1999
- Kang Hui Scholarship for Highest Scorer in High School Entrance Exam, Hangzhou, China, 1996

Patents

1. *Magnetic resonance imaging systems and methods for optimized parallel receive, excite, and shim (oPRES)*
   Hui Han, Yi Wang, John Stager, Junghun Cho, and **Dong Zhou**, pending

Publications

1. *A Robust Crystal Structure Prediction Method to Support Small Molecule Drug Development with Large Scale Validation and Prospective Studies*
   D. Zhou, I. Bier, B. Santra, L. Jacobson, C. Wu, P. Skrdla, P. Devine, H. Yu, R. Abel, R. Friesner, L. Wang, ChemRxiv. (2024); submitted to Nature Communications, doi:10.26434/chemrxiv-2024-f17zp

2. *Quantitative susceptibility mapping of magnetic quadrupole moments*
   J. Cho, **D. Zhou**, Y. Kee, P. Spincemaille, and Y. Wang, Concepts Magn Reson Part A, 7174937 (2019)

3. *Cardiac Quantitative Susceptibility Mapping (QSM) for Heart Chamber Oxygenation*
   Y. Wen, T.D. Nguyen, Z. Liu, P. Spincemaille, **D. Zhou**, A. Dimov, Y. Kee, K. Deh, J. Kim, J. Weinsaft, and Y. Wang, Magn Reson Med 79 (3), 1545 (2018)

4. *Quantitative Susceptibility Mapping (QSM)-Based Cerebral Metabolic Rate of Oxygen Mapping with Minimum Local Variance*
   J. Zhang, J. Cho, **D. Zhou**, T.D. Nguyen, P. Spincemaille, A. Gupta, and Y. Wang, MRM 79 (1), 172 (2018)

5. *Susceptibility underestimation in a high susceptibility phantom: dependence on imaging resolution, magnitude contrast and other parameters*
   D. Zhou, J. Zhang, P. Spincemaille, Y. Wang, Magn Reson Med, 78 (3), 1080 (2017)

6. *Preconditioned Total Field Inversion (TFI) Method for Quantitative Susceptibility Mapping*
   Z. Liu, Y. Kee, **D. Zhou**, Y. Wang, and P. Spincemaille, Magn Reson Med 78 (1), 303 (2017)

7. *Cerebral Metabolic Rate of Oxygen (CMRO2) Mapping with Hyperventilation Challenge using Quantitative Susceptibility Mapping (QSM)*
   J. Zhang, **D. Zhou**, T.D. Nguyen, P. Spincemaille, A. Gupta, Y. Wang, Magn Reson Med, 77 (5), 1762 (2017)

8. *Three-dimensional MR Phase Unwrapping via Dual Decomposition*
   J. Dong, F. Chen, **D. Zhou**, T. Liu, Z. Yu, and Y. Wang, Magn Reson Med 77 (3), 1353 (2017).

9. *On the influence of zero-padding on the nonlinear operations in Quantitative Susceptibility Mapping*
   S. Eskreis-Winkler, **D. Zhou**, T. Liu, A. Gupta, S. A. Gauthier, Y. Wang, and P. Spincemaille, MRI 35, 154 (2017)

10. *Quantitative susceptibility mapping and R2* measured changes during white matter lesion development in multiple sclerosis: myelin breaking down, myelin debris degradation and removal, and iron accumulation*
    Y. Zhang, S.A. Gauthier, A. Gupta, W. Chen, J. Comunale, G.C.-Y. Chiang, **D. Zhou**, G. Askin, W. Zhu, D. Pitt, Y. Wang, AJNR 37 (9) 1629 (2016).

11. *Longitudinal change in magnetic susceptibility of new enhanced multiple sclerosis (MS) lesions measured on serial quantitative susceptibility mapping (QSM)*
    Y. Zhang, S.A. Gauthier, A. Gupta, J. Comunale, G. C.-Y. Chiang, **D. Zhou**, W. Chen, A.E. Giambrone, W. Zhu, Y. Wang, JMRI 44 (2) 426 (2016).

12. *Increase in magnetic susceptibility after MS lesion formation and potential diagnostic utility*
    Y. Zhang, S. Gauthier, L. Tu, A. Gupta, J. Comunale, G.C.-Y. Chiang, **D. Zhou**, Y. Wang, Multiple Sclerosis Journal 21 502 (2016).

13. *Simultaneous Phase Unwrapping and Removal of chemical Shift (SPURS) using Graph Cuts: Application in Quantitative Susceptibility Mapping*
    J. Dong, T. Liu, F. Chen, **D. Zhou**, A. Dimov, A. Raj, Q. Cheng, P. Spincemaille, and Y. Wang, IEEE TMI 34 (2) 531 (2015).

14. *Background field removal by solving the Laplacian boundary value problem*
    D. Zhou, T. Liu, P. Spincemaille, and Y. Wang, NMR in Biomedicine, 27 (3), 312 (2014).

15. *An Iterative Spherical Mean Value (iSMV) Method for Background Field Removal in MRI*
    Y. Wen, **D. Zhou**, T. Liu, P. Spincemaille, and Y. Wang, Magn Reson Med 72 (4) 1065 (2014).

16. *Magnetic susceptibility anisotropy: cylindrical symmetry from macroscopically ordered anisotropic molecules and accuracy of MRI measurements using few orientations*
    C. Wisnieff, T. Liu, P. Spincemaille, S. Wang, **D. Zhou**, and Y. Wang, NeuroImage 70, 363 (2013).

17. *Mediated gates between spin qubits*
    J. Fei, **D. Zhou**, Y.-P. Shim, S. Oh, X. Hu, and M. Friesen, Phys. Rev. A 86, 062328 (2012). arXiv:1207.6063

18. *Cavity-assisted quantum bath engineering with a superconducting qubit*
    K. W. Murch, U. Vool, **D. Zhou**, S. J. Weber, S.M. Girvin, and I. Siddiqi, Phys. Rev. Lett. 109, 163602 (2012); arXiv:1207.0053

19. *Phenomenological noise model for superconducting qubits: two-state fluctuators and 1/f noise*
    D. Zhou and R. Joynt, Supercond. Sci. Techno. 25, 045003 (2012); arXiv:1102.5766

20. *Topology of entanglement evolution of two qubits*
    D. Zhou, G.-W. Chern, J. Fei, and R. Joynt, Int. J. Mod. Phys. B 26, 1250054 (2012); arXiv:1007.1749

21. *Disappearance of entanglement: a topological point of view*
    D. Zhou and R. Joynt, QIP 11, 571 (2012); arXiv:1006.5474

22. *Suppression of decoherence and disentanglement by the exchange interaction*
A. De, A. Lang, **D. Zhou**, and R. Joynt, Phys. Rev. A 83, 042331 (2011); arXiv:1006.5943

23. *Quasi-Hamiltonian Method for Computation of Decoherence Rates.*
R. Joynt, **D. Zhou** and Q.-H. Wang, Int. J. Mod. Phys. B 25, 2115 (2011); arXiv:0906.2843

24. *Noise-induced looping on the Bloch sphere: Oscillatory effects in dephasing of qubits subject to broad-spectrum noise.*
D. Zhou and R. Joynt, Phys. Rev. A 81, 010103 (2010); arXiv:0907.0463

25. *Nacre Protein Fragment Templates Lamellar Aragonite Growth*
RA Metzler, JS Evans, CE Killian, **D Zhou**, TH Churchill, N Appathurai, SN Coppersmith, PUPA Gilbert, J. Am. Chem. Soc. 132, 6329-6334 (2010).

26. *X-ray photoelectron emission spectromicroscopic analysis of arborescent lycopsid cell wall composition and Carboniferous coal ball preservation.*
C. K. Boyce, M. Abrecht, **D. Zhou**, and P.U.P.A. Gilbert, Int. J. Coal Geol. 83, 146-153 (2010).

27. *Disentanglement and decoherence from classical non-Markovian noise: Random telegraph noise.*
D. Zhou, A. Lang, and R. Joynt, QIP 9, 727 (2010); arXiv:0912.3313

28. *Two-particle quantum walks applied to the graph isomorphism problem.*
J. Gamble, M. Friesen, **D. Zhou**, R. Joynt, and S.N. Coppersmith, Phys. Rev. A 81, 052313 (2010); arXiv:1002.3003

29. *A high-resolution chemical and structural study of framboidal pyrite formed within a low-temperature bacterial biofilm.*
L.C.W. MacLean, T. Tyliszczak, P.U.P.A. Gilbert, **D. Zhou**, T.J. Pray, T.C. Onstott, G. Southam. Geobiology 6, 471-480 (2008).

30. *Gradual Ordering in Red Abalone Nacre.*
P.U.P.A. Gilbert, R. A. Metzler, **D. Zhou**, A. Scholl, A. Doran, A. Young, M. Kunz, N. Tamura, S. N. Coppersmith. J. Am. Chem. Soc. 130, 17519-17527 (2008); arXiv:0710.4573

31. *Assignment of polarization-dependent peaks in carbon K-edge spectra from biogenic and geologic aragonite.*
D. Zhou, R.A. Metzler, T. Tyliszczak, J. Guo, M. Abrecht, S.N. Coppersmith, P.U.P.A. Gilbert. J. Phys. Chem. B 112, 13128-13135 (2008).

32. *Probing the organic-mineral interface in model biominerals.*
R. A. Metzler, I.-W. Kim, K. Delak, J.S. Evans, **D. Zhou**, E. Beniash, F. Wilt, M. Abrecht, J.-W. Chiou, J. Guo, S.N. Coppersmith, P.U.P.A. Gilbert. Langmuir 24, 2680-2687 (2008).

33. *Polarization-dependent imaging contrast in abalone shells.*
R.A. Metzler, **D. Zhou**, M. Abrecht, J.-W. Chiou, J. Guo, D. Ariosa, S.N. Coppersmith, P.U.P.A. Gilbert. Phys. Rev. B 77, 064110 (2008).