Zeyin Yan

Personal Information	Date of birth	27^{th} June 1990
	Nationality	Chinese
	Gender	Male
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Research Fields Quantum refinement, Protein Structure, *Ab initio* (HF and DFT) computations, charge, spin and momentum densities, density matrices, Quantum Crystallography, Quantum tunnelling, Machine learning Potential

Experience

SUSTech, Shenzhen, China

Senior Research Fellow, Lung Wa CHUNG Group, 2020.12 – Now

- Topic 1: *Quantum Tunnelling under Electric Fields*
- Topic 2: *Quantum Refinement Approaches for Drug-Design using Machine Learning Potential*
- Supervisor: Lung Wa CHUNG, Prof.

SUSTech, Shenzhen, China

Post-doc, Lung Wa CHUNG Group, 2018.11 – 2020.11

- Topic: *Assessment of Multiscale Quantum Refinement Approaches for Metalloproteins*
- Supervisor: Lung Wa CHUNG, Prof.

SUSTech, Shenzhen, China

Visiting Students, Lung Wa CHUNG Group, 2018.05 – 2018.10

- Supervisor: Lung Wa CHUNG, Prof.

Education

CentraleSupélec, Université Paris-Saclay, SPMS, Paris, France

Ph.D., Physic, 2015.01 – 2018.01

- Thesis Topic: *2D Magnetic Momentum Density Reconstruction and Determination of One-Electron Reduced Density Matrix*
- Supervisor: Jean-Michel Gillet, Prof.

Beihang University, Beijing, China

M.S., ECPKN and Telecommunication (Double Major), 2012.09 – 2015.01

- Thesis Topic: *Research of Single-Photon Laser Radar Imaging Technology Based QSI Protocol*
- Supervisor: Jie Chen, Prof.

B.S., ECPKN (Information and Computing Sciences), 2008.09 – 2012.06

- Project Topic: *Research of materials with high thermal but low electric conductivity*
- Supervisor: Hongzhe Tang, A/Prof.

Project

1. Natural Science Foundation of Shenzhen Innovation Committee(2023-2026) Combining machine learning with quantum refinement methods and applications for protein-drug molecular structures 30W Mainly participate (actual application)

Journal Publications

1. Z. Ma, **Z. Yan(joint first authors)**, X. Li, L. W. Chung. Quantum Tunneling in Reactions Modulated by External Electric Fields: Reactivity and Selectivity *The Journal of Physical Chemistry Letters.* 14, 2023.
2. F. Zheng, Y. Yang, S. Wu, S. Zhao, Y. Zhu, H. Su, J. Dai, **Z. Yan**, L. W. Chung and K. M. Wong. Tetracationic Diiridium(II) Complexes with an Unsupported Ir(II)–Ir(II) Bond Empowered by London Dispersion: Experimental and Computational Studies for Structure-Property Relationships *Communications Chemistry.* 5, 2022.
3. **Z. Yan**, X. Li, L. W. Chung. Multiscale Quantum Refinement Approaches for Metalloproteins. *Journal of Chemical Theory and Computation.* 17, 6, 2021.
4. S. Gueddida, **Z. Yan**, Kibalin, I. A. B. Voufack, N. Claiser. M. Souhassou, C. Lecomte, B. Gillon and J.-M. Gillet. Joint refinement model for the spin resolved one-electron reduced density matrix of YTiO3 using polarized neutron diffraction and magnetic Compton scattering data. *The Journal of Chemical Physics.* 148, 9, 2018.
5. S. Gueddida, **Z. Yan**, and J.-M. Gillet., 2018. Development of a joint refinement model for the spin resolved one-electron-reduced density matrix using different data sets. *Acta Crystallographica Section A*, 74(2):131-142, Mar 2018.
6. I.A. Kibalin, **Z. Yan**, A.B. Voufack, S. Gueddida, B. Gillon, A. Gukasov, F. Porcher, A.M. Bataille, F. Morini, N. Claiser and M. Souhassou. Spin density in $YTiO_3$: I. Joint refinement of polarized neutron diffraction and magnetic x-ray diffraction data leading to insights into orbital ordering. *Physical Review B*, 96(5), p.054426, 2017.
7. **Z. Yan**, I.A. Kibalin, N. Claiser, S. Gueddida, B. Gillon, A. Gukasov, A.B. Voufack, F. Morini, Y. Sakurai, M. Brancewicz and M. Itou. Spin density in $YTiO_3$: II. Momentum-space representation of electron spin density supported by position-space results. *Physical Review B*, 96(5), p.054427, 2017.
8. A.B. Voufack, N. Claiser, C. Lecomte, S. Pillet, Y. Pontillon, B. Gillon, **Z. Yan**, J.-M. Gillet, M. Marazzi, A. Genoni and M. Souhassou. When combined X-ray and polarized neutron diffraction data challenge high-level calculations: spin-resolved electron density of an organic radical. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, 73(4), pp.544-549, 2017.
9. N. Bošnjaković-Pavlović, D. Bajuk-Bogdanović, J. Zakrzewska, **Yan, Z.**, I. Holclajtner-Antunović, J.-M. Gillet, and A. Spasojević-de Biré. Reactivity of 12-tungstophosphoric acid and its inhibitor potency toward Na+/K+-ATPase: A combined 31 P NMR study, ab initio calculations and crystallographic analysis. *Journal of Inorganic Biochemistry*, 176, pp.90-99, 2017.

Codes

ONIOM_QR: https://github.com/yanjordan/ONIOM_QR_mod
Cluster_Model_Cry14: https://github.com/yanjordan/Cluster_Model_Cry14

Presentations

- The 8^{th} International Conference on Theory of Atomic & Molecular Clusters (Beijing, China) September 2017
  "Electron representations in phase space by a cluster approach"
  (**Z. Yan**, S. Gueddida, J. M. Gillet)
- CECAM Discussion Meeting Quantum Crystallography: Current Developments and Future Perspectives (Nancy, France) June 2017
  "Quantum Crystallography in Spin-Resolved Phase-Space."
  (S. Gueddida, **Z. Yan**, I. Kibalin, J. M. Gillet)
- Colloque de Recherche Inter Ecoles Centrales (Paris, France) June 2016
  "Quantum modeling of magnetic scattering experiments."
  (**Z. Yan** & J. M. Gillet)

- European Crystallographic Meeting (Basel, Switzerland) September 2016
  "Probability densities in different spaces: when multipolar-atom model is just not enough."
  (J. M. Gillet, **Z. Yan** et al)

Posters

- European Charge Density Meeting (Warsaw, Poland) June 2016
  "One electron properties of $YTiO_3$ refinement from multi experimental and theoretical investigations"
  (**Z. Yan**, J. M. Gillet, et al)
  "Role of the diagonal and extra diagonal terms of the 1-RDM in the responses to an applied electric field"
  (**Z. Yan**, D. Adrien, Cortona. P. & J. M. Gillet)
- L'Association Française de Cristallographie (Marseille, France) July 2016
  "One electron properties of $YTiO_3$ refinement from multi experimental and theoretical investigations"
  (**Z. Yan**, J. M. Gillet, et al)

Summer schools

- (Nancy, France) August 2016
  "Robert F. Stewart school on electron density and related properties"

Skills

Programming: *Fortran, Python, Shell, Matlab, OpenMP, MPI*

Softwares & Programs: *Gaussian09, GaussianView5, CRYSTAL14, ORCA, CP2K, MolPro, Bader, AIMALL, Multiwfn, MoPro, Molekel, Mercury, Vesta, Pymol, Schrödinger, CNS, Polyrate*

Language: Chinese, English, French

Others: Office, Latex, Linux, HPC

References

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