LAN TRAN

Ho Chi Minh City Institute of Physics, Vietnam Academy of Science and Technology
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PROFESSIONAL EXPERIENCES

Research scientist, Head of Department *2021 – present*
Department of Theoretical and Computational Physics,
Ho Chi Minh City Institute of Physics,
Vietnam Academy of Science and Technology

Postdoctoral researcher *2018 – 2021*
Department of Chemistry,
The University of California, Berkeley

Postdoctoral researcher *2015 – 2018*
Departments of Chemistry and Physics,
The University of Michigan, Ann Arbor

Research scientist *2014 – 2015*
Department of Energy and Environment,
Ho Chi Minh City Institute of Physics,
Vietnam Academy of Science and Technology

Research assistant *2010 – 2011*
Department of Novel and Nanostructured Materials,
Ho Chi Minh City Institute of Physics,
Vietnam Academy of Science and Technology

EDUCATION

Ph.D. in Theoretical Chemistry *2011 – 2014*
The Graduate University for Advanced Studies, Japan,
Supervisor: Takeshi Yanai

M.Sc. in Materials Science *2007 – 2010*
Vietnam National University, Hanoi, Vietnam

B.Sc. in Theoretical Physics *2003 – 2007*
Hue University, Hue City, Vietnam

PUBLICATIONS

Corresponding author of 20 papers (marked by the asterisk)

Peer-reviewed papers

1. **L. Tran***, E. Neuscamman,
"Improving excited state potential energy surfaces via optimal orbital shapes",
The Journal of Physical Chemistry A, **124** 8273 (2020)

2. K. T. Williams, Y. Yao, J. Li, L. Chen, H. Shi, M. Motta, C. Niu, U. Ray, S. Guo, R. J. Anderson, J. Li, **L. Tran**, C. N. Yeh, B. Mussard, S. Sharma, F. Bruneval, M. van Schilfgaarde, G. H. Booth, G. K. L. Chan, S. Zhang, E. Gull, D. Zgid, A. Millis, C. J. Umrigar, and L. K. Wagner (Simons Collaboration on the Many-Electron Problem),
"Direct comparison of many-body methods for realistic electronic Hamiltonians",
Physical Review X, **10** 011041 (2020)

3. **L. Tran***, J. A. R. Shea, E. Neuscamman,
"Tracking excited states in wave function optimization using density matrices and variational principles",
Journal of Chemical Theory and Computation, **15** 4790 (2019)

4. L. B. Ho and **L. Tran***,
"Tunable cloaking of Mexican-hat confined states in bilayer silicene",
Communications in Physics, **29** 215 (2019)

5. A. A. Rusakov, S. Iskakov, **L. Tran***, and D. Zgid,
"Self-energy embedding theory (SEET) for periodic systems"
Journal of Chemical Theory and Computation **15** 229 (2018) – **ACS Editor's Choice**

6. D. Nguyen and **L. Tran***,
"Assessment of Electrocatalytic Performance of Metal-Free C-doped BN Nanoflakes for Oxygen Reduction and Hydrogen Evolution Reactions: A Comparative Study",
The Journal of Physical Chemistry C **122** 21124 (2018)

7. **L. Tran***, S. Iskakov, and D. Zgid
"Spin-unrestricted self-energy embedding theory",
The Journal of Physical Chemistry Letters **9** 4444 (2018)

8. **L. Tran*** and D. Zgid,
"Generalized self-energy embedding theory",
The Journal of Physical Chemistry Letters **8** 2200 (2017)

9. **L. Tran***, A. Shee, J. Li, E. Gull, and D. Zgid,
"Testing self-energy embedding theory in combination with GW",
Physical Review B **96** 155106 (2017)

10. M. Motta, D. M. Ceperley, G. K. Chan, J. A. Gomez, E. Gull, S. Guo, C. Jimenez-Hoyos, **L. Tran**, J. Li, F. Ma, A. J Millis, N. V. Prokof'ev, U. Ray, G. E. Scuseria, S. Sorella, E. M. Stoudenmire, Q. Sun, I. S. Tupitsyn, S. R. White, D. Zgid, S. Zhang (Simons Collaboration on the Many Electron Problem),
"Towards the solution of the many-electron problem in real materials: equation of state of the hydrogen chain with state-of-the-art many-body methods",
Physical Review X **7** 031059 (2017) – **Highlighted on Phys.org**

11. **L. Tran***, A. A. Kananenka, and D. Zgid,
"Rigorous ab initio quantum embedding for quantum chemistry using Greens function theory: screened interaction, non-local self-energy relaxation, orbital basis, and chemical accuracy",
Journal of Chemical Theory and Computation **12** 4856 (2016)

12. H. Le, and **L. Tran***,
"Photoenhanced spin/valley polarization and tunneling magnetoresistance in ferromagnetic-

normal-ferromagnetic silicene junction",
Journal of Physics D: Applied Physics **49** 375106 (2016)

13. A. A. Kananenka, A. R. Welden, **L. Tran**, E. Gull, and D. Zgid,
"Efficient temperature-dependent Greens function methods for realistic systems: using cubic spline interpolation to approximate Matsubara Greens functions",
Journal of Chemical Theory and Computation **12** 2250 (2016)

14. **L. Tran***, A. A. Kananenka, and D. Zgid,
"Communication: Towards ab initio self-energy embedding theory in quantum chemistry",
The Journal of Chemical Physics **143** 241102 (2015)

15. **L. Tran***, J. Chalupský, and T. Yanai,
"Molecular g-tensors from analytical response theory and quasi-degenerate perturbation theory in the framework of complete active space self-consistent field method,"
Molecular Physics **113** 1750 (2015) – **Invited paper**

16. **L. Tran***, H. Le, and H. Tran,
"Electronic, magnetic, and spin-polarized transport properties of hybrid graphene/boron-nitride nanoribbons having 5-8-5 line defects at the heterojunction,"
Physica Status Solidi B **252** 573 (2015)

17. T. Yanai, Y. Kurashige, M. Wataru, J. Chalupský, **L. Tran**, and M. Saitow,
"DMRG for ab initio calculations and associated dynamic correlation methods: A review of theory and applications"
International Journal of Quantum Chemistry **115** 283 (2015) – **Invited paper**

18. **L. Tran***, Y. Kurashige, and T. Yanai,
"Scalar reltativistic calculations of hyperfine coupling constants using ab initio DMRG in combination with DKH3 transformation: case studies of 4d transition metals",
Journal of Chemical Theory and Computation **11** 73 (2014)

19. **L. Tran***, Y. Kurashige, and T. Yanai,
"Toward reliable prediction of hyperfine coupling constants using ab initio DMRG method: diatomic $^2\Sigma$ and vinyl radicals as test cases,"
Journal of Chemical Theory and Computation **10** 1953 (2014)

20. Y. Kurashige, J. Chalupský, **L. Tran**, and T. Yanai,
"Complete active space second-order perturbation theory with cumulant approximation for large entanglement space from DMRG",
The Journal of Chemical Physics **141** 174111 (2014)

21. **L. Tran***,
"Electronic transport properties of molecular junctions based on the direct binding of aromatic ring to electrodes,"
Chemical Physics **428** 53 (2014)

22. **L. Tran*** and T. Yanai,
"Correlated one-body potential from MP2 theory: alternative to OO-MP2 method,"
The Journal of Chemical Physics **138** 224108 (2013)

23. H. Le, **L. Tran***, and H. Tran,
"Monte Carlo simulations of core/shell nanoparticles containing interfacial defects: role of

disordered ferromagnetic spins,"
Physica B: Condensed Matter **430** 10 (2013)

24. **L. Tran*** and H. Tran,
"Role of the poly-dispersity and the dipolar interaction in magnetic nanoparticle systems: Monte Carlo study,"
Journal of Non-Crystaline Solids **357**, 996 (2011)

25. H. Tran, L. H. Phuc, L. K. Vinh, B. D. Long, T. T. Kieu, N. N. Bich, **L. Tran**, N. Q. Hien, L. H. A. Khoa, and N. N. V. Tam,
"Immobilizing of anti-HPV18 and E. coli O157: H7 antibodies on magnetic silica-coated Fe_3O_4 for early diagnosis of cervical cancer and diarrhea,"
International Journal of Nanotechology **8**, 383 (2011) – **Highlighted on ScienceDaily and Phys.org**

26. **L. Tran*** and H. Tran,
"Monte Carlo simulation of magnetic nanoparticle systems,"
Computational Materials Science **49**, S287 (2010)

Invited chapters

1. **L. Tran**, H. Tran, L. H. Phuc, L. K. Vinh, T. T. Kieu, and N. Q. Hien,
"Magnetic Nanoparticles: Computer Simulation, Chemical Syntheses, and Biomedical Diagnoses", in book: MAGNETIC NANOPARTICLES: PROPERTIES, SYNTHESES, AND APPLICATIONS, edited by B. Acklin and E. Lautens,
Nova Science Publisher, pp. 297-317 (2012)

2. **L. Tran** and H. Tran,
"Using Monte Carlo Method to Study Magnetic Properties of Frozen Ferrofluid", in book: APPLICATIONS OF MONTE CARLO METHOD IN SCIENCE AND ENGINEERING, edited by S. Mark and S. Mordechai,
INTECH Publisher, pp. 495-512 (2011)

ORAL PRESENTATIONS

1. The University of Illinois at Urbana-Champaign, IL, USA (Jan. 2020)
2. Oak Ridge National Laboratory, TN, USA (Nov. 2019)
3. Pitzer Center for Theoretical Chemistry, UC Berkeley, CA, USA (Sep. 2019)
4. ACS Fall National Meeting, San Diego, CA, USA (Aug. 2019)
5. Pitzer Center for Theoretical Chemistry, UC Berkeley, CA, USA (Sep. 2018)
6. ACS Fall National Meeting, Washington DC, USA (Aug. 2017)
7. The 49^{th} Midwest Theoretical Chemistry Conference, Michigan, USA (Jun. 2017)
8. The 57^{th} Sanibel Symposium, St. Simons Island, Georgia, USA (Feb. 2017)
9. Vietnam–Japan Physics Workshop, Ho Chi Minh City, Vietnam (Nov. 2014)
10. The 36^{th} National Conference on Theoretical Physics, Quy Nhon, Vietnam (Aug. 2011)

STUDENT ADVISING

- Ho B. Le: now a postdoc at Tohoku University;
- Duyen B. Nguyen: now a PhD student at Central Michigan University;
- Working and co-authoring with students at the University of Michigan and the University of California, Berkeley

PREVIOUS GRANTS

- Vietnam National Foundation for Science and Technology Development (NAFOSTED), 2015 (No. 103.01-2015.14)
- Japan's Ministry of Education, Culture, Sports, Science and Technology (MEXT), 2011
- Vietnam National Foundation for Science and Technology Development (NAFOSTED), 2011 (No. 103.022011.11)

AWARDS

The Government (MEXT) Scholarship for Ph.D. study, Japan 2011

Rencontres Du Vietnam, France 2010

COMPUTER PROGRAMMING

Languages and tools

- Fortran, C++, Python, gdb, shell script
- MPI, OpenMP, pthread

Development projects

- Developed the code for tracking excited states during wave-function optimization
- Implemented Krylov iterative and Newton-style codes for excited-state optimizations
- Developed the C++ code of Green's function embedding theory
- Developed the MPI/OpenMP hybrid code of the second-order self-energy evaluation
- Developed the code of self-consistent second-order Møller-Plesset perturbation theory
- Developed Krylov iterative codes for solving the FCI and DMRG linear response equations
- Implemented codes for evaluating electronic paramagnetic resonance (EPR) parameters
- Developed codes of the third-order DKH quasi-relativistic transformation

Source codes

- QMCPack: quantum Monte Carlo methods
- pySCF, TFES (UC Berkeley), Orz (IMS Japan): quantum chemistry methods
- Green (U Michigan): many-body Green's function methods

MISCELLANEOUS

Languages:

- Vietnamese: native
- English: fluent
- Japanese: beginning

Scientific activities:

- Reviewer of *Nanoscale, Physical Chemistry Chemical Physics, Journal of Magnetism and Magnetic Materials, The Journal of Physical Chemistry*
- Member of *Vietnam Theoretical Physics Society (VTPS)* since 2009.
- Member of *American Chemistry Society (ACS)* since 2017