QUOC DAI HO

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OBJECTIVE

Seeking a challenging position in theoretical and computational modeling of energy-related materials. Using my expertise in first-principles electronic structure calculations and computational chemistry/materials science, I aim to contribute to innovative research at the intersection of chemistry, physics, and materials science. My goal is to support the development of next-generation sustainable energy solutions through advanced simulations and close collaboration with experimentalists.

EDUCATION

- **Department of Materials Science and Engineering, University of Delaware** *2019 – early 2025 (expected)*
  Ph.D. in Materials Science and Engineering Newark, Delaware, United States
  ◦ GPA: 3.80/4.00
- **University of Science and Technology** *2015 – 2017*
  Master in Nanomaterials Science and Engineering Seoul, Republic of Korea
  ◦ GPA: 4.07/4.50. Percentage equivalent 95.22/100
- **Department of Chemistry, Quy Nhon University** *2008 – 2012*
  Bachelor in Chemistry Quy Nhon, Vietnam
  ◦ GPA: 8.55/10.00. Salutatorian

RECENT PROJECTS

- **Project 1: Controlling spin dynamics in altermagnets by strong coupling** *2024 – Present*
  Tools: VASP, Wannier90, OpenMX, TB2J, analytical tight-binding model [GitHub]
  ◦ Searching for materials having magnon quasiparticles with THz functionality within the new phase of magnetism dubbed altermagnets (AM)
  ◦ Studying the strong coupling between magnons in AM with other quasiparticles forming hybridized quasiparticles such as phonon-plasmon-magnon polaritons.
  ◦ Ultimately controlling spin dynamics in AM by external perturbations such as light or thermal sources.
- **Project 2: Spontaneous Development of Surface Magnetism in RuO_2** *2023 – Present*
  Tools: VASP, LOBSTER, HIVE-STM, VESTA [GitHub]
  ◦ Demonstrated the emergence of surface magnetization at the (110) surface of non-magnetic bulk RuO_2
  ◦ Explained the phenomenon through surface symmetry breaking caused by termination, leading to structural modifications and electronic reconstruction.
  ◦ Showed that surface magnetism in RuO_2(110) generates spin-polarized surface states, spin-resolved STM images, and potential spin-dependent transport phenomena.
- **Project 3: Electronic Structures of Rare-Earth Pnictides Under Dimensionality Reduction** *2021 – 2023*
  Tools: VASP, OpenMX, Wannier90, WannierTools, VESTA [GitHub]
  ◦ Investigated the electronic structure of semi-metallic rare-earth monopnictide (RE-V) thin films using first-principles hybrid functional calculations, focusing on LaSb as a case study
  ◦ Discovered the quantum spin Hall (QSH) insulator phase in ultrathin (001)-oriented films (3, 5, 7 monolayers), with a band inversion driven by selective effect of quantum confinement on electron and hole bands near Fermi level and a topological gap opened by spin–orbit coupling
  ◦ Demonstrated that RE-V thin films can exhibit topological properties, with potential for coupling 4f magnetism with nontrivial band structures in ultrathin films.
- **Project 4: Electronic Structures of Rare-Earth Pnictides Under Strain** *2021 – 2023*
  Tools: VASP, OpenMX, Wannier90, WannierTools, `chinook`, VESTA [GitHub]
  ◦ Investigated the evolution of band topology in biaxially strained GdSb(001) epitaxial films using ARPES and DFT, demonstrating strain-induced tuning of bandgaps in rare-earth monopnictides
  ◦ Developed a tight-binding model explaining orbital-specific band shifts and the role of biaxial compressive strain in promoting band inversion and increasing electron carrier density
  ◦ Highlighted practical implications for strain-controlled topological phase transitions and semimetal-semiconductor transitions, paving the way for advanced applications in magnetic Weyl semimetals and topological half-Heusler alloys.

SKILLS

- **Programming Languages:** Python, Mathematica, Shell scripting
- **Research Software:** VASP, Quantum ESPRESSO (QE), OpenMX, Gaussian, LOBSTER, Wannier90, TB2J, etc.

GRANTED PROJECTS

- **The Korea Institute of Science and Technology School Partnership Project program** *2018, 2019*
  Korea Institute of Science and Technology
  - Data driven search for highly efficient 3d transition (bi)metallic sulfides-based (photo)-electrochemical catalysts (2018, PI).
  - Investigation of (photo)electrocatalytic properties of monolayer MoS_2 modified by sulfur vacancy and transition metals doping (2019, PI).

HONORS AND AWARDS

- **Graduate Student Travel Award** *2022, 2025*
  Graduate College, University of Delaware
  - Supported by the Office of the Provost to help University of Delaware graduate students participate in significant professional conferences.
  - Opportunities for presenting student work in a professional setting and for networking and exposure to the latest academic research.
- **Gold Medalist in Vietnam National Chemistry Olympiad for University Students** *2010, 2012*
  Chemical Society of Vietnam
  - Achieved national rankings: 7th out of 142 participants in 2010 (as a sophomore) and 3rd out of 139 in 2012 (as a senior).
  - Demonstrated expertise in General, Analytical, Inorganic, Organic, and Physical Chemistry, covering both advanced theoretical knowledge and fundamental experimental skills.
- **Odon Vallet Scholarships for Academic and Research Excellence** *2006, 2007, 2010, 2012*
  The Vallet Scholarship Fund
  - Prestigious scholarship awarded to outstanding students with excellent academic and research achievements.
  - Recognized for consistent academic excellence and contribution to research over multiple years.
- **Annual Government Scholarship for Excellent Students** *2008 – 2012*
  Ministry of Education, Vietnam
  - Merit-based scholarship awarded to top-performing students nationwide, recognizing exceptional academic records.
  - Supported undergraduate studies, enabling opportunities for further research and professional development.

REFERENCES

1. **Anderson Janotti**
   Professor, Department of Materials Science and Engineering
   University of Delaware, Newark, Delaware, United States
   Email: janotti@udel.edu
   Relationship: PhD thesis advisor
2. **Garnett W. Bryant**
   Group leader, Nanoscale Device Characterization Division
   National Institute of Standards and Technology, Gaithersburg, Maryland, United States
   Professor, Joint Quantum Institute
   University of Maryland, College Park, Maryland, United States
   Email: garnett.bryant@nist.gov
   Relationship: Co-advisor and thesis committee member
3. **Matthew F. Doty**
   Professor, Department of Materials Science and Engineering
   University of Delaware, Newark, Delaware, United States
   Email: doty@udel.edu
   Relationship: Thesis committee member and experimentalist collaborator

PUBLICATIONS

For an updated list of publication please visit my homepage

1. D. Quang To, **Dai Q. Ho**, Joshua M. O. Zide, Lars Gundlach, M. Benjamin Jungfleisch, Garnett W. Bryant, Anderson Janotti, and Matthew F. Doty, Tunable magnon band topology and magnon orbital Nernst effect in noncollinear antiferromagnets, **2025** (In preparation)

2. Igor Evangelista, Intuon Chatratin, Muhammad Zubair, Ruiqi Hu, **Dai Q. Ho**, Abdul Saboor, Shoaib Khalid, Ioanna Fampiou, Anderson Janotti, Effects of Uniaxial Strain on the Electronic Structure of Transition-Metal Dichalcogenides, **2025** (In preparation)

3. Muhammad Zubair, **Dai Q. Ho**, D. Quang To, Shoaib Khalid, Anderson Janotti, Topological Weyl semimetals phase and intrinsic spin Hall conductivity in $Sb_{1-x}As_x$ and $Bi_{1-x}As_x$ alloys, **2025** (In preparation)

4. **Dai Q. Ho**, D. Quang To, Ruiqi Hu, Garnett W. Bryant, Anderson Janotti, Symmetry breaking induced surface magnetization in non-magnetic RuO_2, **2025** (To be submitted) link

5. Muhammad Hassan Shaikh, Matthew Whalen, **Dai Q. Ho**, Aqiq Ishraq, Collin Maurtua, Kenji Watanabe, Takashi Taniguchi, Yafei Ren, Anderson Janotti, John Xiao, and Chitraleema Chakraborty, Magnetic proximity coupling to defects in a two-dimensional semiconductor, **2025** (under revision at *ACS Nano*) link

6. Ruiqi Hu, **Dai Q. Ho**, D. Quang To, Garnett W. Bryant, Anderson Janotti, Fermi Level Pinning in ErAs Nanoparticles Embedded in III-V Semiconductors, *Nano Lett.*, **2024**, 24, 15, 4376-4382 link.

7. Nguyen Ngoc Tri, **Dai Q. Ho**, Nguyen Tien Trung, Theoretical insights into the adsorption and gas sensing performance of Fe/Cu doped graphene, *Phys. Chem. Chem. Phys.*, **2024**, 26, 14265-14276 link

8. Nguyen Ngoc Tri, **Dai Q. Ho**, Nguyen Tran Gia Bao, Nguyen Tien Trung, The adsorption of tetracycline, ciprofloxacin on reduced graphene oxide surfaces: role of intermolecular interaction, *Chemical Physics*, **2024**, 579, 112207 link

9. **Dai Q. Ho**, Ruiqi Hu, D. Quang To, Garnett W. Bryant, Anderson Janotti, Emerging nontrivial topology in ultra-thin films of rare-earth pnictides, *ACS Nano*, **2023**, 17, 21, 20991–20998 link

10. Hadass S. Inbar, **Dai Q. Ho***, Shouvik Chatterjee, Aaron N. Engel, Shoaib Khalid, Connor P. Dempsey, Mihir Pendharkar, Yu Hao Chang, Shinichi Nishihaya, Alexei V. Fedorov, Donghui Lu, Makoto Hashimoto, Dan Read, Anderson Janotti, Christopher J. Palmstrøm, Tuning the band topology of GdSb by epitaxial strain, *APL Materials*, **2023**, 11, 111106 (*co-first author) link

11. Tran Nam Trung, Nguyen Thi Thuy Kieu, **Dai Q. Ho**, Dong-Bum Seo, Eui-Tae Kim, Understanding the doping mechanism of Sn in TiO_2 nanorods toward efficient photoelectrochemical performance, *Journal of Materials Science*, **2023**, 58 (5), 2156-2169 link

12. Hadass S. Inbar, **Dai Q. Ho**, Shouvik Chatterjee, Mihir Pendharkar, Aaron N. Engel, Jason T. Dong, Shoaib Khalid, Yu Hao Chang, Taozhi Guo, Alexei V. Fedorov, Donghui Lu, Makoto Hashimoto, Dan Read, Anderson Janotti, and Christopher J. Palmstrøm, Epitaxial growth, magnetoresistance, and electronic band structure of GdSb magnetic semimetal films, *Phys. Rev. Materials*, **2022**, 6 (12), L121201 link

13. Yongchen Liu, Wilder Acuna, Huairuo Zhang, **Dai Q. Ho**, Ruiqi Hu, Zhengtianye Wang, Anderson Janotti, Garnett Bryant, Albert V. Davydov, Joshua M. O. Zide, Stephanie Law, Bi_2Se_3 Growth on (001) GaAs Substrates for Terahertz Integrated Systems, *ACS Appl. Mater. Interfaces*, **2022**, 14 (37), 42683-42691 link

14. D. Quang To, Zhengtianye Wang, **Dai Q. Ho**, Ruiqi Hu, Wilder Acuna, Yongchen Liu, Garnett W. Bryant, Anderson Janotti, Joshua M. O. Zide, Stephanie Law, and Matthew F. Doty, Strong coupling between a topological insulator and a III-V heterostructure at terahertz frequency, *Phys. Rev. Materials*, **2022**, 6 (3), 035201 link

15. Nguyen Ngoc Tri, **Dai Q. Ho**, A. J. P. Carvalho, Minh Tho Nguyen, Nguyen Tien Trung, Insights into adsorptive interactions between antibiotic molecules and rutile-TiO_2(110) surface, *Surface Science*, **2021**, 703, 121723 link

16. Nguyen Thi Thanh Cuc, **Dai Q. Ho**, Nguyen Thi Ai Nhung, Nguyen Phi Hung, Nguyen Tien Trung, Roles of H_2O to hydrogen bonds, structure and strength of complexes of CH_3CHS and H_2O, *Vietnam Journal of Chemistry*, **2019**, 57 (4), 425-432 link

17. Pham N. Khanh, Cam-Tu D. Phan, **Dai Q. Ho**, Quan Van Vo, Vu T. Ngan, Minh T. Nguyen, and Nguyen T. Trung, Insights into the Cooperativity between Multiple Interactions of Dimethyl Sulfoxide with Carbon Dioxide and Water, *Journal of Computational Chemistry*, **2019**, 40 (2), 464-474 link

18. Nguyen Ngoc Tri, **Dai Q. Ho**, Nguyen Tien Trung, Insights into the absorption of organic molecules on rutile TiO_2(110) surface: A theoretical study, *Vietnam Journal of Chemistry*, **2018**, 56 (6), 751-756 link

19. **Dai Q. Ho**, Seungchul Kim, Role of Aluminum Doping in Anatase to Rutile Transformation from Thermodynamic View Point, *Phys. Status Solidi RRL*, **2018**, 12 (12), 1800234 link

20. **Dai Q. Ho**, Nguyen Ngoc Tri, Nguyen Thi Thu Trang, and Nguyen Tien Trung, Remarkable effects of substitution on stability of complexes and origin of the C-H$\cdots$O(N) hydrogen bonds formed between acetone's derivative and CO_2, XCN (X = F, Cl, Br), *RSC Adv.*, **2014**, 4, 13901-13908 link