Quoc Dai Ho

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EDUACATION

✓ **Aug 2019 – now**
Department of Materials Science and Engineering
University of Delaware, Newark, Delaware, United States
PhD candidate in Materials Science and Engineering

✓ **Mar 2015 – Aug 2017**
University of Science and Technology, Daejeon, Republic of Korea
Korea Institute of Science and Technology campus, Seoul, Republic of Korea
Master of Nanomaterials Science and Engineering

✓ **Sep 2008 – Jun 2012**
Quy Nhon University, Quy Nhon, Binh Dinh, Vietnam
B.S., Department of Chemistry

ACADEMIC EXPERIENCE

Aug 2019 – now
Ph.D. candidate | Department of Materials Science and Engineering, University of Delaware, Newark, DE, USA

- First-principles calculations applied in materials science
- DFT and tight binding simulation for quantum materials
- DFT calculations of defect physics in semiconductors

Mar 2015 – Aug 2017
Master Student | Computational Science Research Center, KIST, Department of Nanomaterials Science and Engineering, Korea University of Science and Technology

- DFT calculations of defect physics in semiconductors
- High throughput DFT calculations for electrochemical catalyst screening

Aug 2014 – Oct 2014
Visiting Scholar | Faculty of Science, KU Leuven, Belgium

- High performance computing system management
- Quantum chemical calculation

Jul 2012 – Feb 2015
Lecturer and Researcher | Department of Chemistry, Quy Nhon University

- Lecturer in Physical and Theoretical Chemistry
- Studying the nature of blue-shifting hydrogen bond, interactions between CO_2 and carbonyl/thiocarbonyl model organic molecules

RESEARCH INTERESTS

- First-principles calculations and (semi)empirical calculations applied in materials science
- DFT calculations for materials discovery, particularly for electronic devices, quantum technology, energy transformation, and catalysts
- Quantum chemical calculations for bonding and reaction in chemistry

Granted project

- Data driven search for highly efficient 3d transition (bi)metallic sulfides based (photo)-electrochemical catalysts (Principal Investigator, KIST school partnership project, 2018)
- Investigation of (photo)electrocatalytic properties of monolayer MoS_2 modified by sulfur vacancy and transition metals doping (Principal Investigator, KIST school partnership project, 2019)

SKILLS

Computational

- Operating systems: Unix/Linux, Windows
- Programming languages: Python, Fortran
- Softwares: VASP, Quantum Expresso, Gaussian, AIM 2000, NBO, VESTA, Gaussview, Molden, Origin, Corel Draw, GNUplot, matplotlib, etc.

Excellent teamwork skills

PUBLICATIONS

1. 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 (**IF 2.3**)
2. **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 (**IF 17.1**)
3. 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, Strain Tuning the Band Topology of Epitaxial GdSb Quantum Wells, *APL Materials*, **2023**, 11, 111106 ([*]co-first author) **(IF 6.1)**
4. 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 **(IF 4.5)**
5. 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 **(IF 3.4)**

6. 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 **(IF 9.5)**
7. 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 **(IF 3.4)**
8. 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 **(IF 1.9)**
9. Nguyen Thi Thanh Cuc, **Ho Quoc Dai**, 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 **(IF 0.9)**
10. 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 **(IF 3.0)**
11. Nguyen Ngoc Tri, **Ho Quoc Dai**, Nguyen Tien Trung, Chemisorption of enrofloxacin on rutile-TiO_2 (110) surface: a theoretical investigation, *Vietnam J. Sci. Technol.*, **2019**, 57(4), 449–456
12. Truong Tan Trung, Phan Dang Cam Tu, **Ho Quoc Dai**, Nguyen Phi Hung, Nguyen Tien Trung, A theoretical study on interaction and stability of complexes between dimethyl sulfide and carbon dioxide, *Quy Nhon University Journal of Science*, **2019**, 13 (1), 95-105
13. Nguyen Ngoc Tri, **Ho Quoc Dai**, 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 **(IF 0.9)**
14. **Dai Q. Ho** and Seungchul Kim, Role of Aluminum Doping in Anatase-to-Rutile Transformation from Thermodynamic View Point, *Phys. Status Solidi RRL*, **2018,** 12 (12), 1800234 **(IF 2.8)**
15. Nguyen Ngoc Tri, Pham Thi Minh Tam, Nguyen Thi Hong Man, **Ho Quoc Dai**, Nguyen Phi Hung, Nguyen Tien Trung, Interactions of formaldehyde and its substituted derivatives with HCN: Structure, stability and interaction. *Vietnam Journal of Chemistry*, **2016**, 54(4), 448-453 (**IF 0.9**)
16. Nguyen Khoa Hien, Nguyen Thi Ai Nhung, **Ho Quoc Dai**, Nguyen Tien Trung, Duong Tuan Quang, A Fluorescent sensor based on Dansyl Diethylenetriamine

Thiourea conjugate: a thorough theoretical investigation, *Vietnam Journal of Chemistry*, **2015**, 53 (5e), 541-546 **(IF 0.9)**

17. **Ho Quoc Dai**, 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···O(N) hydrogen bonds formed between acetone's derivative and CO_2, XCN (X = F, Cl, Br), *RSC Adv.*, **2014**, 4, 13901-13908 **(IF 3.9)**

Submitted preprints and in preparation

1. Ruiqi Hu, **Dai Q. Ho**, D. Quang To, Garnett W. Bryant, Anderson Janotti, Fermi level pinning in ErAs nanoparticles embedded in III-V semiconductors (under review at *Nano Letters*) arXiv:2312.12184v1
2. Nguyen Ngoc Tri, **Dai Q. Ho**, Nguyen Tien Trung, Insights into the adsorption and gas sensing performance of Fe/Cu doped graphene (submitted to *Applied Surface Science*)
3. Muhammad Zubair, **Dai Q. Ho**, Shoaib Khalid, Anderson Janotti, Topological Weyl semimetals and alloys (in preparation)
4. 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 (TMD) (in preparation)

HONOR and AWARDS

- Odon Vallet scholarships for excellent academic and research performance in the years of 2006, 2007, 2010, and 2012
- Annual Government Scholarship for Excellent Students, 2008 – 2012
- 3rd prize in the 6th Vietnam National Chemistry Olympiad competition for University Student, Chemical Society of Vietnam (CSV), 2010
- 1st prize in the 7th Vietnam National Chemistry Olympiad competition for University Student competition, Chemical Society of Vietnam (CSV), 2012