

BIOGRAPHICAL SKETCH

IDENTIFYING INFORMATION:

Name: Duy Le

Position title: Assistant Scientist

Mailing Address: 4111 Libra Drive, Physical Sciences Bldg. 430, Orlando, FL 32816-2385

Tel: 407-823-2325 Email; duy.le@ucf.edu

(a) Professional Preparation:

ORGANIZATION AND LOCATION	DEGREE (if applicable)	DATE RECEIVED	FIELD OF STUDY
University of Central Florida, Orlando, FL, USA	Postdoctoral Fellow	2012 - 2016	Physics
University of Central Florida, Orlando, FL, USA	PHD	05/2012	Physics
Ho Chi Minh University of Pedagogy, Ho Chi Minh, VIETNAM	BS	08/2002	Physics

(b) Appointments and Positions

- 05/2019 – Present Secondary Joint Appointment, Renewable Energy & Chemical Transformations cluster, University of Central Florida.
- 11/2016 – Present Assistant Scientist, Department of Physics, University of Central Florida.
- 08/2002 – 08/2004 Lecturer, Department of Physics, Ho Chi Minh City University of Pedagogy, Vietnam.

(c) Products

Products that are the most current ones related to your field

1. Le D. An Explicit-Implicit Hybrid Solvent Model for Grand Canonical Simulations of the Electrochemical Environment. ChemRxiv 2023. Available from: <https://doi.org/10.26434/chemrxiv-2023-z2n4n> DOI: 10.26434/chemrxiv-2023-z2n4n
2. Le D, Rahman TS. On the role of metal cations in CO₂ electrocatalytic reduction. Nature Catalysis. 2022; 5(11):977-978. Available from: <https://doi.org/10.1038/s41929-022-00876-2> DOI: 10.1038/s41929-022-00876-2
3. Tan W, Xie S, Le D, Diao W, Wang M, Low K, Austin D, Hong S, Gao F, Dong L, Ma L, Ehrlich S, Rahman TS, Liu F. Fine-tuned local coordination environment of Pt single atoms on ceria controls catalytic reactivity. Nature Communications. 2022; 13(1):7070. Available from: <https://doi.org/10.1038/s41467-022-34797-2> DOI: 10.1038/s41467-022-34797-2
4. Rawal T, Le D, Hooshmand Z, Rahman T. Toward alcohol synthesis from CO hydrogenation on Cu(111)-supported MoS₂ – predictions from DFT+KMC. The Journal of Chemical Physics. 2021; 154(17):174701. Available from: <https://doi.org/10.1063/5.0047835> DOI: 10.1063/5.0047835
5. Wasim E, Din N, Le D, Zhou X, Sterbinsky GE, Pape MS, Rahman T S, Tait SL. Ligand-coordination effects on the selective hydrogenation of acetylene in single-site Pd-ligand supported catalysts. Journal of Catalysis. 2022; 413:81-92. Available from: <https://doi.org/10.1016/j.jcat.2022.06.010> DOI: 10.1016/j.jcat.2022.06.010

Other Significant Products

1. Le D, Rawal T, Rahman T. Single-Layer MoS₂ with Sulfur Vacancies: Structure and Catalytic Application. *The Journal of Physical Chemistry C*. 2014; 118(10):5346-5351. Available from: <https://doi.org/10.1021/jp411256g> DOI: 10.1021/jp411256g
2. Kersell H, Hooshmand Z, Yan G, Le D, Nguyen H, Eren B, Wu C, Waluyo I, Hunt A, Nemšák S, Somorjai G, Rahman T, Sautet P, Salmeron M. CO Oxidation Mechanisms on CoO_x-Pt Thin Films. *Journal of the American Chemical Society*. 2020; 142(18):8312-8322. Available from: <https://doi.org/10.1021/jacs.0c01139> DOI: 10.1021/jacs.0c01139
3. Nash D, Restrepo D, Parra N, Giesler K, Penabade R, Aminpour M, Le D, Li Z, Farha O, Harper J, Rahman T, Blair R. Heterogeneous Metal-Free Hydrogenation over Defect-Laden Hexagonal Boron Nitride. *ACS Omega*. 2016; 1(6):1343-1354. Available from: <https://doi.org/10.1021/acsomega.6b00315> DOI: 10.1021/acsomega.6b00315
4. Rawal T, Acharya S, Hong S, Le D, Tang Y, Tao F, Rahman T. High Catalytic Activity of Pd₁/ZnO(10 $\bar{1}$ 0) toward Methanol Partial Oxidation: A DFT+KMC Study. *ACS Catalysis*. 2018; 8(6):5553-5569. Available from: <https://doi.org/10.1021/acscatal.7b04504> DOI: 10.1021/acscatal.7b04504
5. Posysaev S, Miroshnichenko O, Alatalo M, Le D, Rahman T. Oxidation states of binary oxides from data analytics of the electronic structure. *Computational Materials Science*. 2019; 161(15):403-414. Available from: <https://doi.org/10.1016/j.commatsci.2019.01.046> DOI: 10.1016/j.commatsci.2019.01.046

(d) Graduate teaching experience

- NONE

(e) Graduate students mentored (to completion, if applicable)

- NONE

(f) Other synergistic activities related to Graduate Education

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| 2023 | Develop a computational methodology for first principles simulation of the electrochemical system. |
| 2021-2023 | Co-Organizing symposium “Electrocatalysis for Sustainable Energy: Fundamental, Applications, & Perspective” for ACS National Meeting, Fall 2021, 2022, 2023 |
| 2022 | Co-Organizing focus session “Computational Design and Discovery of Novel Materials” for APS March Meeting 2022 |
| 2023 | Associate member of the Committee on Community Activities of the American Chemical Society |
| 2020-2022 | Chair-Elect, Chair, Immediate-past Chair of the ACS Orlando Local Section: Led the Orlando Section to its first-ever ChemLuminary Award; Chemist Celebrate Earth Day Coordinator (2021-2023); Developed the website (https://orlandoacs.org) for the Orlando Section; Currently serving as the webmaster; Member of SERMACS2025 Organizing Committee. |