Curriculum Vitae

Hung M. Le, Ph.D.
Head of Division of Material Modeling
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Research Expertise

Computational Material Modeling, Numerical Fitting, Theoretical Reaction and Collision Dynamics.

Education

B.S. in Chemistry, University of Central Oklahoma, Edmond, Oklahoma (2005).
Ph.D. in Computational Chemistry, Oklahoma State University, Stillwater, Oklahoma (2009).

Professional Appointments

2016 – present: Senior Scientist, Division of Molecular Modeling, Center for Innovative Materials and Architectures Vietnam National University.
2010 – 2015: Faculty Member, Faculty of Materials Science, University of Science, Vietnam National University.
2013 – 2014: Visiting Scholar, Division of Chemistry and Biological Chemistry, Nanyang Technological University.
2010: Postdoctoral researcher at Institute for Shock Physics, Washington State University.
2006 – 2009: Research Assistant, Department of Chemistry, Oklahoma State University.

Publications (*corresponding author)

(26 published papers, 228 citations with Hirsch index of 9 according to Researchgate.com)

26. Thi H. Ho, Viet Q. Bui, Thang Bach Phan, Yoshiyuki Kawazoe, **Hung M. Le***, "Atomistic observation of the collision and migration of Li on $MoSe_2$ and WS_2 surfaces through ab initio molecular dynamics", *Phys. Chem. Chem. Phys.* 19, 27332 (2017).
25. Nguyet N. T. Pham, **Hung M. Le***, "A density functional theory investigation of Ni_n, Pd_n, Pt_n Clusters (n=1-4) adsorbed on buckminsterfullerene (C_{60})", *ChemPhysChem* 18, 1376 (2017).
24. Hieu T. Nguyen-Truong, **Hung M. Le***, Yoshiyuki Kawazoe, Duc Nguyen-Manh, "Ab initio direct dynamics of transition metal atom/dimers bombardments onto graphene", *Carbon* 115, 791 (2017).
23. Thi H. Ho, Hieu C. Dong, **Hung M. Le***, Yoshiyuki Kawazoe, "Effect of elasticity of the MoS_2 surface on Li atom bouncing and migration: Mechanism from ab initio molecular dynamic investigations", *J. Phys. Chem. C* 121, 1329 (2017).
22. **Hung M. Le***, Vo Duy Dat, Tan-Tien Pham, Yoshiyuki Kawazoe, "First-principles modeling of metal(II) ferrocyanide: Electronic property, magnetism, bulk moduli, and the role of $C{\equiv}N^-$ defect", *J. Phys. D* 50, 035004 (2016).
21. Viet Q. Bui, **Hung M. Le***, Yoshiyuki Kawazoe, Yongho Kim*, "Adjusting band gap and charge transfer of organometallic complex adsorbed on MoS_2 Monolayer using vertical electric-field: A first-principles investigation", *J. Phys. Condens. Matter* 29, 015003 (2016).
20. **Hung M. Le***, Viet Q. Bui, Phuong H. Tran, Nguyen-Nguyen Pham-Tran, Yoshiyuki Kawazoe, Duc Nguyen-Manh, "The prospect of sensitizing organic dyes attached to the MoS_2 surface: Physical insights from density functional theory investigations", *Chem. Phys. Lett.* (2016).
19. **Hung M. Le***, Tan-Tien Pham, Thach S. Dinh, Yoshiyuki Kawazoe, Duc Nguyen-Manh, "First-principles modeling of 3D-transition-metal-atom adsorptions on silicene: A linear-response DFT+U approach", *J. Phys. Condens. Matter* 28, 135301 (2016).
18. Thi H. Ho, Nguyen-Nguyen Pham-Tran, Yoshiyuki Kawazoe, **Hung M. Le***, "An ab initio investigation of O-H dissociation from the Al-OH_2 complex using molecular dynamics and neural network fitting", *J. Phys. Chem. A* 120, 346 (2016).
17. Viet Q. Bui, Tan-Tien Pham, Duy A. Le, Thi M. Cao, **Hung M. Le***, "A first-principles investigation of various gas (CO, H_2O, NO, and O_2) adsorptions on a WS_2 monolayer: Stability and electronic properties", *J. Phys. Condens. Matter* 27, 305005 (2015).
16. Hieu T. Nguyen-Truong, **Hung M. Le***, "An implementation of the Levenberg-Marquardt algorithm for simultaneous-energy-gradient fitting using two-layer feed-forward neural networks", *Chem. Phys. Lett.* 629, 40 (2015).
15. **Hung M. Le***, Wilson K. H. Ng, Hajime Hirao*, "Electronic and magnetic properties of C_{60}-Fe_n-graphene intercalating nanostructures (n=1-6) predicted from first-principles calculations", *Chem. Phys. Lett.* 618, 127 (2015).
14. Viet Q. Bui, **Hung M. Le***, "Naphthalene adsorptions on graphene using $Cr/Cr_2/Fe/Fe_2$ linkages: Stability and spin perspectives from first-principles calculations", *Chem. Phys. Lett.* 614, 238 (2014).

13. **Hung M. Le***, Hajime Hirao*, Yoshiyuki Kawazoe, Duc Nguyen-Manh, "Nanostructures of C_{60}-metal-graphene (metal = Ti, Cr, Mn, Fe, or Ni): A spin-polarized density functional theory study", *J. Phys. Chem. C* 118, 21057 (2014).
12. **Hung M. Le***, Nam H. Vu, Bach-Thang Phan*, "Migrations of oxygen vacancy in tungsten oxide (WO_3): A density functional theory study", *Comput. Mater. Sci.* 90, 171 (2014).
11. Viet Q. Bui, Tan-Tien Pham, Hoai-Vu S. Nguyen, **Hung M. Le***, "Transition metal (Fe and Cr) adsorptions on buckled and planar silicene monolayers: A density functional theory investigation", *J. Phys. Chem. C* 117, 23364 (2013).
10. **Hung M. Le***, Hajime Hirao, Yoshiyuki Kawazoe, Duc Nguyen-Manh, "First-principles modeling of C_{60}–Cr–graphene nanostructures for supporting metal clusters", *Phys. Chem. Chem. Phys.* 15, 19395 (2013).
9. Hieu T. Nguyen-Truong, Thi M. Cao, **Hung M. Le***, "Theoretical investigations of BBS→BSB transformation on an ab initio potential energy surface obtained from neural network fitting", *Chem. Phys.* 426, 31 (2013).
8. Viet Q. Bui, **Hung M. Le***, Yoshiyuki Kawazoe, Duc Nguyen-Manh, "Graphene-Cr-graphene intercalation nanostructures: Stability and magnetic properties from density functional theory investigations", *J. Phys. Chem. C* 117, 3605 (2013).
7. Nam H. Vu, Hieu V. Le, Thi M. Cao, Viet V. Pham, **Hung M. Le***, Duc Nguyen-Manh, "Anatase-rutile phase transformation of titanium dioxide (TiO_2) bulk material: A DFT+U approach", *J. Phys. Condens. Matter* 24, 405501 (2012).
6. Hieu T. T. Nguyen, **Hung M. Le***, "Modified feed-forward neural network structures and combined-function-derivative approximations incorporating exchange symmetry for potential energy surface fitting", *J. Phys. Chem. A* 116, 4629 (2012).
5. Anh T. H. Le, Nam H. Vu, Thach S. Dinh, Thi M. Cao, **Hung M. Le***, "Molecular dynamics investigations of chlorine peroxide dissociation on a neural network ab initio potential energy surface", *Theor. Chem. Acc*. 131, 1158 (2012).
4. **Hung M. Le***, Thach S. Dinh, Hieu V. Le, "Molecular dynamics investigations of ozone on an ab initio potential energy surface with the utilization of pattern-recognition neural network for accurate determination of product formation", *J. Phys. Chem. A* 115, 10862 (2011).
3. **Hung M. Le** and Lionel M. Raff*, "Theoretical investigation of BeH + H_2→BeH_2 + H using classical dynamics on an ab initio potential energy surface obtained from neural network fitting", *J. Phys. Chem. A* 114, 45 (2010).
2. **Hung M. Le**, Sau Huynh, and Lionel M. Raff*, "Molecular dissociation of hydrogen peroxide on a neural network ab initio potential surface with a new configuration sampling method involving gradient fitting", *J. Chem. Phys.* 131, 014107 (2009).
1. **Hung M. Le** and Lionel M. Raff*, "Cis→trans, trans→cis isomerizations and N–O bond dissociation of nitrous acid (HONO) on an ab initio potential surface obtained by novelty sampling and feed-forward neural network fitting", *J. Chem. Phys.* 128, 194310 (2008).

Research Projects

3/2017 – current: "Examining electronic and magnetic properties of graphene, MoS_2, WS_2 monolayers interacting with metal and gas-storage capability of $[CoFe(CN)_6]^{2-}$ using DFT calculations" (PI, grant **103.01-2016.53** from NAFOSTED).
4/2015 – 3/2016: "Theoretical investigations of organic dyes/conductive polymers adsorptions on a MoS_2/WS_2 monolayer", Department of Materials Science, Vietnam National University (PI, project **hp150037** awarded by HPCI Office, Japan).
3/2014 – 2/2016: "Development of artificial neural network construction to construct a force field for graphene", Department of Material Science, Vietnam National University (PI, grant **B2014-18-03** from VNU).
3/2014 – 2/2016: "Developing *ab initio* potential energy surfaces for $(H_2O)_n^+$ systems using neural network fitting" (PI, grant **103.01-2013.28** from NAFOSTED).
08/2013 – 8/2014: "Designing new graphene-based materials for catalysis", Division of Chemistry and Biological Chemistry, Nanyang Technological University, Singapore (participant).
1/2011 – 7/2013: "Theoretical investigation of anatase-rutile phase transition in TiO_2 crystal using molecular dynamics simulation", Department of Materials Science, Vietnam National University (PI, grant **B2012-18-10-TĐ** from VNU).
1/2010 – 8/2010: "High pressure invesitgations of RDX structures and reaction pathways in the condensed phase using a hybrid QM:QM scheme." Supervisor: Dr. Santanu Chaudhuri (Institute for Shock Physics, Washington State University).
8/2006 – 9/2009: "Neural network fitting in *ab initio* potential surface development." Supervisor: Prof. Lionel M. Raff (Oklahoma State University).

Teaching Experience

General Chemistry Laboratory, Department of Chemistry, Oklahoma State University.
Group Theory, Faculty of Materials Science, University of Science, Vietnam National University.
Quantum Physics, Faculty of Materials Science, University of Science, Vietnam National University.
Electronic Structure Calculations in Materials Science, Faculty of Materials Science, University of Science, Vietnam