

Curriculum Vitae

PHALGUN LOLUR

Missouri University of Science and Technology
120B, Schrenk Hall, Department of Chemistry
400 West 11th Street
Rolla, MO 65409-0010
phalgun.lolur@mst.edu

Education:

Ph. D., Chemistry – Missouri University of Science and Technology. 2011 – 2015 (expected).

- Theoretical chemistry for spectroscopy and dynamics (Dr. Richard Dawes).

M.S., Chemical Engineering – Missouri University of Science and Technology. 2010 – 2013.

- Modeling global potential energy surfaces (Dr. Richard Dawes and Dr. Daniel Forciniti).

B.Tech., Chemical Engineering – Vellore Institute of Technology. 2006 – 2010.

Skills

High Accuracy Quantum Chemistry

- Global and multi-state potential energy calculations using multi-reference methods – MOLPRO, Gaussian
- Complete basis set (CBS), energy component extrapolation methods
- Explicitly correlated methods – CCSD(T)-F12, MRCI-F12
- Spin-orbit and derivative coupling

Theoretical dynamics using potential energy surfaces

- DVR calculations of bound and resonant ro-vibrational states
- Vibronic states on coupled potential energy surfaces
- Quasi-classical trajectories (QCT) – VENUS code

Mathematical scripting and data processing

- Linear algebra matrix and eigenvalue optimization – MATLAB and Mathematica
- Visualization, plotting and 3D printing – MATLAB, Plotly, Blender, Solidworks
- Completed MATLAB programming workshops – developed visual interactive apps to demonstrate kinetics

Image and video processing for illustrations and figures

- Photoshop, GIMP, Irfanview, Picasa, Cyberlink PowerDirector, Sony Vegas

Publications

1. Phalgun Lolur, Richard Dawes, Michael Heaven "Theoretical Studies of Vibronic Perturbations in Magnesium Carbide", *Mol. Phys.* (Accepted. DOI: 10.1080/00268976.2015.1087601)
2. Phalgun Lolur, Richard Dawes, Silver Nyambo, Cyrus Karshenas, Scott A. Reid, "Towards a Global Model of Spin-Orbit Coupling in the Halocarbenes", *J. Chem. Phys.* **142** (21), 214304 (2015).
3. Phalgun Lolur, Richard Dawes, "3D Printing of Molecular Potential Energy Surface Models" *J. Chem. Ed.* **91**, 1181 (2014).
4. Richard Dawes, Phalgun Lolur, Anyang Li, Bin Jiang and Hua Guo, "An accurate global potential energy surface for the ground state of ozone", *J. Chem. Phys.* **139**, 201103 (2013).
5. Chong Tao, Craig Richmond, Calvin Mukarakate, Scott H. Kable, George B. Bacskay, Eric C. Brown, Richard Dawes, Phalgun Lolur and Scott A. Reid, "Spectroscopy and dynamics of the predissociated, quasi-linear S_2 state of chlorocarbene" *J. Chem. Phys.*, **137**, 104307/1-104307/8 (2012).
6. Richard Dawes, Phalgun Lolur, Jianyi Ma and Hua Guo, "Highly Accurate Ozone Formation Potential and Implications for Kinetics", *J. Chem. Phys.*, **135**, 081102 (2011).

Presentations and Posters

1. A theoretical study of vibronic perturbations in magnesium carbide (MgC), Poster presentation, 25th Dynamics of Molecular Collisions conference (Asilomar, CA, July 12-17, 2015).
2. Modeling spin-orbit coupling in the halocarbenes, Research talk, 70th International Symposium for Molecular Spectroscopy (Champaign, IL, June 22-26, 2015).
3. Studying the vibronic perturbations in magnesium carbide, Poster presentation, Graduate Research Showcase (Missouri S&T, Rolla, MO, April 1, 2015).
4. *Ab initio* Quantum Chemistry: From Approach to Applications, Research talk, Chemistry department (Missouri S&T, Rolla, MO, February 23, 2015).
5. Highly accurate potential energy surface calculations for spectroscopy and dynamics, Research talk, Université Montpellier 2 (Montpellier, France, November 25, 2014).
6. Highly accurate potential energy surface calculations for spectroscopy and dynamics, Research talk, Université de Reims Champagne-Ardenne (Reims, France, November 19, 2014).
7. Vibronic perturbations in magnesium carbide, Poster presentation, Mid-West Regional ACS Meeting (Columbia, MO, November 14, 2014).
8. Vibronic perturbations in the electronic spectrum of MgC, Research talk, 69th International Symposium for Molecular Spectroscopy (Champaign, IL, June 16-20, 2014).

9. Reduction of BOD in dairy industries, Research talk, ChemInsight conference (Indian Institute of Technology, Kharagpur, West Bengal, India, March 13-15, 2009).
10. Ocean thermal energy conversion systems, Poster presentation, Gravitass engineering conference (Vellore Institute of Technology, Vellore, Tamil Nadu, India, September 11-13, 2009).
11. The curious case of feline aerodynamics, Abstract idea talk, Equilibria conference (Vellore Institute of Technology, Vellore, Tamil Nadu, India, January 07-09, 2008).
12. Protection of Communication Devices from Solar Flares, Proposal talk, Students for Exploration and Development of Space (SEDS) International Conference (Vellore Institute of Technology, Vellore, Tamil Nadu, India, September 22-23, 2007).
13. Sat Card, Business proposal talk, Students for Exploration and Development of Space (SEDS) International Conference (Vellore Institute of Technology, Vellore, Tamil Nadu, India, September 22-23, 2007).

Educational software for public use

1. Developed software (interactive apps) to demonstrate chemical reaction kinetics for various reactions using Matlab.
2. Developed software to create 3D STL files for 3D printing potential energy surfaces from raw data using Matlab and Excel.

Internships

- | | | |
|----|--------------------------------|------|
| 1. | Honeywell Technology Solutions | 2010 |
| 2. | Visaka Industries Limited | 2009 |
| 3. | INOX - Air Products | 2008 |

Accolades

1. Received the best graduate student poster presentation award at Dynamics of Molecular Collisions (DMC) 2015.
2. Referee for journal of chemical education (ACS publications).
3. Sorter for the American Physical Society's national meeting at San Antonio in March 2015.
4. Completed Ph. D. candidacy in Fall 2014.
5. Achieved the honor's list status at Missouri S&T in Fall 2014.
6. Received VPGS Scholar's award of \$7,000 from the office of graduate studies to pursue Ph. D. studies in 2012.

7. Runner-up for Donald D. Myers scholarship which recognizes Missouri S&T students who made an impact on the campus and community through involvement and service in 2011.
8. Recognized as an active volunteer of the "Rebuild Joplin" program in 2011.
9. Awarded the first prize for the 'Transforma' event, which involved transforming of one working model into another during 'Pragyan 2008' at NIT, Tiruchirappalli.
10. Secured the second position for the event 'le Code X', which involved solving chemical engineering problems through C, C++ and FORTRAN during 'Equilibria' at VIT, Vellore in 2008.
11. Secured second position for the event 'Scratch Pad', an abstract idea presentation event during 'Equilibria' at VIT, Vellore in 2008.
12. Secured second position in a collage competition on 'ill effects of tobacco' at VIT, Vellore in 2008.
13. Awarded the fourth prize for a contraption event, which involved maximizing energy conversions to solve a given problem during 'Pragyan 2008' at NIT, Tiruchirappalli.
14. Successfully completed the CCNA (Cisco Certified Network Associate) exploration course offered by CISCO, which covered the basic networking concepts in 2008.

Organized Events/Conferences/Workshops

1. Organizer for the Celebration of Nations events in Rolla during 2010, 2011 and 2012.
2. Event coordinator for the International Students' Day in 2011.
3. Chief organizer for the events Holi and Diwali in 2011.
4. Coordinator for organizing the event 'Diwali' for the Indian Association at Missouri S&T in 2010
5. Board member of the Mars Rover competition at SEDS Indian National Conference, SINC -10, held at VIT, Vellore.
6. Chief organizer of Riviera' 09, an International Sports and Cultural Festival, held at VIT, Vellore.
7. Board member of Programme committee, which was responsible for organizing the events at SEDS Indian National Conference, SINC-09, held at VIT, Vellore. Organized the event called "Lunar Trek", where bots were pitted against each other to solve the given problem statement in a moon-like terrain.
8. Coordination officer for "gravitas" 09, an international knowledge carnival, held at VIT, Vellore. Organized the event called "Delta T", which involved the design of an insulation chamber to minimize the temperature drop of the given fluid.
9. Design coordinator for the "International Conference on Advances in Mechanical and Building Sciences", an international conference held at VIT, Vellore during December 09.

Campus Involvement

1. Volunteered as a grad student representative for prospective students for office of graduate studies and societies like Omega Chi Epsilon.
2. Part of the search committee for hiring an assistant director of Career Opportunities & Employer Relations in 2014.
3. Part of the campus grievances committee for Missouri University of Science and Technology for the years 2012-2014.
4. Treasurer and Secretary for the Freethinker's Philosophy Club for the year 2013-2014.
5. Vice-President of Taekwondo martial arts club for the year 2013.
6. Vice- President of the Council of Graduate Students for the year 2011-2012.
7. Multimedia Head for the India Association for the year 2011.
8. Event Coordinator and the student council representative for the International Students' Club for the year 2010-2011.
9. Department representative of Chemical Engineering for the Council of Graduate Students for the year 2010-2011.

References

Dr. Richard Dawes

Associate Professor, Chemistry Department
120C Schrenk Hall
Missouri University of Science and Technology
Rolla, MO 65409-0010
(573) 341-4451
dawesr@mst.edu

Dr. Jeffrey G. Winiarz

Associate Professor, Chemistry Department
332 Schrenk Hall
Missouri University of Science and Technology
Rolla, MO 65409-0010
(573) 341-6733
winiarzi@mst.edu

Dr. Yanzhi Zhang

Assistant Professor, Math and Statistics Department
110 Rolla Building
Missouri University of Science and Technology
Rolla, MO 65409-0010
(573) 341-4651
zhangyanz@mst.edu