Han Guo

Email address: hanguo@chem.umass.edu

Cell phone: 413-801-9761

SKILLS

- **Programming**: Fortran, C, Python, MPICH/Open MPI, Linux script
- **Modeling**: Ab Initio Modeling, Quantum Dynamics, Numerical Analysis
- **Software and tools**: VASP, GAUSSIAN 09, Microsoft Office, VMD, Jmol, VESTA, GaussView
- **Operating systems**: Linux, Mac/OS, Windows
- **Languages**: Mandarin, English

EDUCATION

Ph.D. (2013-present) **University of Massachusetts Amherst, MA, USA**: program in physical chemistry
GPA: 3.86/4. Courses included advanced physical chemistry, statistical thermodynamics, quantum chemistry, mathematical statistics, online courses in Python and machine learning, etc.

M.S. (2009-2012) **Sichuan University, Chengdu, China**: program in physical chemistry
GPA: 90.71/100, 3.64/4. Courses included computational chemistry, mathematics in quantum mechanics, Peking university summer school in Quantum Mechanics (Ⅱ), etc.

B.S. (2005-2009) **Sichuan University, Chengdu, China**: program in general chemistry
GPA: 86.80/100, 3.46/4

RESEARCH EXPERIENCE

Sep 2013 - present Research Assistant, University of Massachusetts Amherst, USA

Project: Theoretical study of the reaction dynamics of methane on metal surfaces using a quantum mechanical approach based on the Reaction Path Hamiltonian (RPH)

- Implemented new methods and codes for the RPH-based quantum scattering approach; e.g. the use of a revised force-projected Hessian, the treatments for lattice motion, the models for rotational motion, and so on. Programmed in Fortran.
- Performed scattering calculations to understand the reaction dynamics and the mode- and bond-selectivity in the dissociation of methane and its isotopologues on smooth metal surfaces. Behaviors are explained in terms of symmetry, mode-softening and nonadiabatic transitions between different vibrationally adiabatic states.
- Developed a model to understand the mode specificity observed in the dissociative sticking of methane excited to four stretch overtone and combination states of different vibrational symmetry.
- Investigated the effects of lattice motion on methane dissociation on different metal surfaces.
- Collaborated with an experimental group studying methane dissociation on the stepped Pt(211) surface. Performed electronic structure calculations and quantum scattering calculations. Good agreement between theory and experiment is observed.
- Investigated the effects including van der Waals interactions when modeling methane dissociation, and tested the accuracy of a new SRP-DFT functional.

Sep 2007 - Jun 2012 Research Assistant, Sichuan University, China

Project: Computational study on CuI-catalyzed ligand-free N-arylation of imidazole with bromobenzene

- Used DFT method to construct two reaction paths for the full catalytic cycle.
- Performed Intrinsic Reaction Coordinate (IRC) analysis and frequency analysis for the optimized transition states and local minima. Identified the optimum path by free energy analysis.
- Applied CPCM-solvent model to investigate catalytic reactions in DMF solvent.

PUBLICATIONS

1. E. A. High, N. Chen, Y. Huang, A. L. Utz*, **H. Guo** and B. Jackson*, "Mode- and Bond-Selectivity in the Dissociation of CH_2D_2 (ν_1 and ν_6 C–H Stretch) on Ni(111)", manuscript in preparation.
2. H. Chadwick, **H. Guo**, A. Gutiérrez-González, J. P. Menzel, B. Jackson and R. D. Beck, "Methane Dissociation on the Steps and Terraces of Pt(211) Resolved by Quantum State and Impact Site", *The Journal of Chemical Physics*, 148, 014701 (9 pages) (2018), chosen as a Featured Article. The American Institute of Physics has issued a press release based on this article.
3. D. Migliorini, H. Chadwick, F. Nattino, A. Gutiérrez-González, E. Dombrowski, E. A. High, **H. Guo**, A. L. Utz, B. Jackson, R. D. Beck and G. J. Kroes, "Surface Reaction Barriometry: Methane Dissociation on Flat and Stepped Transition-Metal Surfaces", *The Journal of Physical Chemistry Letters*, 8, 4177-4182 (2017).
4. P. M. Hundt, M. E. van Reijzen, R. D. Beck*, **H. Guo** and B. Jackson*, "Quantum-State-Resolved Reactivity of Overtone Excited CH_4 on Ni(111): Comparing Experiment and Theory", *The Journal of Chemical Physics*, 146, 054701 (8 pages) (2017).
5. **H. Guo** A. Farjamnia, and B. Jackson, "Effects of Lattice Motion on Dissociative Chemisorption: Toward a Rigorous Comparison of Theory with Molecular Beam Experiments", *The Journal of Physical Chemistry Letters*, 7, 4576-4584 (2016). Featured on the cover of *The Journal of Physical Chemistry Letters*.
6. **H. Guo** and B. Jackson, "Mode-Selective Chemistry on Metal Surfaces: The Dissociative Chemisorption of CH_4 on Pt(111)", *The Journal of Chemical Physics*, 144, 184709 (10 pages) (2016).
7. V. L. Campbell, N. Chen, **H. Guo**, B. Jackson and A. L. Utz, "Substrate Vibrations as Promoters of Chemical Reactivity on Metal Surfaces", *The Journal of Physical Chemistry A*, 119, 12434-12441 (2015).
8. **H. Guo** and B. Jackson, "Mode- and Bond-Selective Chemistry on Metal Surfaces: The Dissociative Chemisorption of CHD_3 on Ni(111)", *The Journal of Physical Chemistry C*, 119, 14769-14779 (2015).
9. **H. Guo**, and Y. Xue, "Theoretical Study on CuI-Catalyzed Ligand-Free N-Arylation of Imidazole with Bromobenzene", *Journal of Theoretical and Computational Chemistry*, 11, 1135-1147 (2012).

SELECTED POSTERS AND PRESENTATIONS

- H. Guo and B. Jackson, "Dissociative Chemisorption of Methane on Ni(111) and Pt(111)", poster presented at ResearchFest, UMass Amherst, MA (2016).
- H. Guo and B. Jackson, "Mode- and Bond-Selective Chemistry on Metal Surfaces: The Dissociative Chemisorption of Methane on Ni(111) and Pt(111)", poster presented at Dynamics at Surfaces Gordon Research Conference, Newport, RI (2015).

HONORS AND AWARDS

2015	Travel Award: Dynamics at Surfaces Gordon Research Conference, Newport, RI
2009—2012	Second Grade Scholarship of Sichuan University
2009	Longsheng Scholarship
2009	Excellent Undergraduate Thesis Award
2009	Excellent Undergraduate Student Award
2008	First Prize of "Scientific Innovation Challenge of Sichuan University"
2007	Excellent Student Award

OTHER EXPERIENCE

Teaching Assistant

General Chemistry Lab Physical Chemistry Lab General Chemistry lecture teaching assistant