

Dr. Lei Liu

Nationality: Chinese

Date of Birth: 28th, Sep. 1983

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Address: Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany



Education

2010,08–2015,03 Ph.D. (with distinction), Computational Chemistry, Jacobs University, Germany

2007,09–2010,07 M.Sc., Applied Chemistry, Research Institute of Petroleum Processing, China

2003,09–2007,07 B.Sc., Applied Chemistry, Beijing Institute of Petrochemical Technology, China

Professional Experience

2017,05- present Postdoctoral researcher, Max Planck Institute for Polymer Research, Germany

2015,05-2017,04 Postdoctoral researcher, University of Bonn, Germany

Research Interests and Expertise

My research interests are in computational chemistry, mainly the application of density functional theory and ab initio molecular dynamics simulations. Research topics include:

- 1) electronic structures of atomic clusters;
- 2) reaction mechanism for homogeneous catalysis;
- 3) computational catalyst design;
- 4) capture and conversion of small molecules.

Professional Services

Editor Board: *J. Appl. Theor.*

Reviewer: *Angew. Chem. Int. Ed.*; *ACS Catal.*; *J. Chem. Theory Comput.*; *Phys. Chem. Chem. Phys.*; *RSC Adv.*

Committee: International Conference on Advanced Energy Materials; International Conference on Energy Materials and Applications.

Honors and Awards

2015 PhD with special distinction

2014 DAAD PhD Fellowship

2013 Marie Curie Visiting Fellowship

2009 Graduate Student Research Fellowship

Completed Publications

I, Book Chapters

- 3 Latest researches in the supports and active component of hydrodesulfurization (HDS) catalyst. In **Hot Topics in Petroleum Processing Technology**. Editor-in-chief: S.B. Tian. Chemical Industry Press: Beijing, **2012**, ISBN: 9787122122391 (in Chinese)
- 2 Progress of research on modification of vegetable oils as lubricant-oil. In **Hot Topics in Petroleum Processing Technology**. Editor-in-chief: S.B. Tian. Chemical Industry Press: Beijing, **2012**, ISBN: 9787122122391 (in Chinese)
- 1 Polyurea lubricating grease. In **Lubricating Grease Technology (Second Edition)**. Editor-in-chief: Y.B. Zhu. China Petrochemical Press: Beijing, **2009**, ISBN: 9787511400871 (in Chinese)

II, Peer-Reviewed Journal Papers (* indicating corresponding author)

- 27 L.F. Gong, W. Li, E. Osorio, X.M. Wu, T. Heine, **L. Liu**.* The effects of halogen elements on the opening of an icosahedral B₁₂ framework. *J. Chem. Phys.*, **2017**, 147 (14), 026738
- 26 **L. Liu**, J.G. Brandenburg, S. Grimme. On the hydrogen activation by frustrated Lewis pairs in solid state: benchmark studies and theoretical insights. *Phil. Trans. R. Soc. A*, **2017**, 375 (2101), 20170006
- 25 K. Bamford, L. Longobardi, **L. Liu**, S. Grimme, D.W. Stephan. FLP reduction and hydroborations of phenanthrene o-iminoquinones and α -diimines. *Dalton. Trans.*, **2017**, 46 (16), 5308-5319
- 24 L. Longobardi, P. Zatsepin, R. Korol, **L. Liu**, S. Grimme, D.W. Stephan. Reactions of boron-derived radicals with nucleophiles. *J. Am. Chem. Soc.*, **2017**, 139 (1), 426-435
- 23 **L. Liu**.* B. Lukose, B. Ensing.* Hydrogen activation by frustrated Lewis pairs revisited by metadynamics simulations. *J. Phys. Chem. C*, **2017**, 121 (4), 2046-2051
- 22 **L. Liu**.* E. Osorio, T. Heine. Understanding the central location of a hexagonal hole in a B₃₆ cluster. *Chem. Asian J.*, **2016**, 11 (22), 3220-3224
- 21 **L. Liu**.* B. Lukose. Geometries and electronic structures of boron clusters: planar Structures and all-boron fullerenes. *J. Apl. Theol.*, **2016**, 1 (2), 5-8
- 20 S. Jalife, **L. Liu**, S. Pan, J. L. Cabellos, E. Osorio, T. Heine, K. J. Donald, G. Merino. Dynamical behavior of boron clusters. *Nanoscale*, **2016**, 8 (40), 17639-17644
- 19 F. Tsao, A. E. Waked, C. Levy, H. Jordan, **L. Liu**, S. Grimme, D. W. Stephan. S(VI) Lewis acids: fluorosulfoxonium cations. *Chem. Commun.*, **2016**, 52 (84), 12418-12421
- 18 T. Özgün, K. Bergander, **L. Liu**, G. Kehr, C. G. Daniliuc, S. Grimme, G. Erker. A frustrated phosphane-borane Lewis pair and hydrogen: a kinetics study. *Chem. Eur. J.*, **2016**, 22 (34), 11958-11961
- 17 K. Ye, G. Kehr, C. G. Daniliuc, **L. Liu**, S. Grimme, G. Erker. Coupling of carbon monoxide with nitrogen monoxide at a frustrated Lewis pair template. *Angew. Chem. Int. Ed.*, **2016**, 55 (32), 9216-9219
- 16 **L. Liu**.* E. Osorio, T. Heine.* The importance of dynamics studies on sandwich structures: a CrB₂₄ case. *Phys. Chem. Chem. Phys.*, **2016**, 18 (27), 18336-18341
- 15 T. Wang, G. Kehr, **L. Liu**, S. Grimme, C. G. Daniliuc, G. Erker. Selective oxidation of an active intramolecular amine/borane frustrated Lewis pair with dioxygen. *J. Am. Chem. Soc.*, **2016**, 138 (13), 4302-4305
- 14 T. Wang, **L. Liu**, S. Grimme, G. Kehr, C. G. Daniliuc, G. Erker. Cyclic Amine/borane Lewis Pairs by the Reaction of N,N-Diallylaniline with Lancaster's H₂B-C₆F₅ Reagent. *Chem. Asian J.*, **2016**, 11 (9), 1394-1399
- 13 T. Özgün, K. Ye, C. G. Daniliuc, B. Wibbeling, **L. Liu**, S. Grimme, G. Kehr, G. Erker. Why does the intramolecular trimethylene-bridged frustrated Lewis pair Mes₂PCH₂CH₂CH₂B(C₆F₅)₂ not activate dihydrogen? *Chem. Eur. J.*, **2016**, 22 (17), 5988-5995
- 12 L. Longobardi, **L. Liu**, S. Grimme, D.W. Stephan. Stable borocyclic radicals via frustrated Lewis pair hydrogenations. *J. Am. Chem. Soc.*, **2016**, 138 (8), 2500-2503
- 11 **L. Liu**.* N. Vankova, T. Heine. A kinetic study on the reduction of CO₂ by frustrated Lewis pairs: from unraveling to rational design. *Phys. Chem. Chem. Phys.*, **2016**, 18 (5), 3567-3574
- 10 **L. Liu**.* D. Moreno, E. Osorio, A. C. Castro, S. Pan, P. K. Chattaraj, T. Heine,* G. Merino.* Structure and bonding of IrB₁₂⁻: converting a rigid boron B₁₂ Platelet to a Wankel Motor. *RSC Adv.*, **2016**, 6 (32), 27177-27182
- 9 **L. Liu**, P. Petkov, T. Heine, G. Rösenthaler, J. Eicher, N. Vankova. Are intramolecular frustrated Lewis pairs also intramolecular catalysts? A theoretical study on H₂ activation. *Phys. Chem. Chem. Phys.*, **2015**, 17 (16): 10687-10698
- 8 M. Fagiani, **L. Liu**, T. Esser, D. Gabel, T. Heine, K. Asmis, J. Warneke. Opening of an icosahedral boron framework: a combined infrared spectroscopic and computational study. *Chem. Phys. Lett.*, **2015**, 625: 48-52
- 7 D. Moreno, S. Pan, **L. Liu**, R. Islas, E. Moreno, G. Martínez-Guajardo, P. K. Chattaraj, T. Heine, G. Merino. B₁₈²⁻: a quasi-planar bowl member of the wankel motor family. *Chem. Commun.*, **2014**, 50 (60): 8140-8143
- 6 **L. Liu**, N. Vankova, A. Mavrantakis, T. Heine, G. V. Rösenthaler, J. Eicher. On the mechanism of hydrogen activation by frustrated Lewis pairs. *Chem. Eur. J.*, **2013**, 19 (51): 17413-17424
- 5 **L. Liu**, N. Vankova, C. Knapp, D. Gabel, T. Heine. On the gas-phase dimerization of negatively charged close-dodecaborates: a theoretical study. *Phys. Chem. Chem. Phys.*, **2013**, 15 (25): 10358-10366
- 4 P. Farràs, N. Vankova, **L. Liu**, J. Warneke, T. Dülcks, T. Heine, C. Viñas, F. Teixidor, D. Gabel. From icosahedron to a plane - flattening dodecaido-dodecaborate by successive stripping of iodine. *Chem. Eur.*

- J.*, **2012**, 18 (41): 13208–13212
- 3 T. C. Nugent, A. Sadiq, A. Bibi, T. Heine, **L. Liu**, N. Vankova, B. S. Bassil. Noncovalent bifunctional organocatalysts: powerful tools for contiguous quaternary–tertiary stereogenic carbon formation, scope and origin of enantioselectivity. *Chem. Eur. J.*, **2012**, 18 (13):4088–4098
 - 2 **L. Liu**, H.W Sun. Multi–step synthesis and properties of tetraurea grease. *Ind. Lubric. Tribol.*, **2011**, 63 (6): 453–455
 - 1 **L. Liu**, H.W Sun. Impact of polyurea structure on grease properties. *Lubr. Sci.*, **2010**, 22 (9):405–413

III, Issued Patents (first authors)

- 6 8–uril grease lubricant and its preparation method. CN102417854B
- 5 Hexaurea lubricating grease and preparation method thereof. CN102417843B
- 4 Tetra–urea lubricating grease and preparation method thereof. CN102382707B
- 3 Carbonyl octoamine compound and preparation method thereof. CN102372654B
- 2 Carbonylhexamine compound and preparation method thereof. CN102372656B
- 1 Carbonyl tetraamine compound and preparation method thereof. CN102372655B

IV, Invited Talks

- 2017-09 “computational studies on the hydrogen activation by frustrated Lewis pairs in solid state”
2017 CAS-TWAS Symposium on Green Chemistry and Technology for Sustainable Development, Beijing, China
- 2017-05 “computations: from atomic clusters to molecular crystals”
The 2nd South Lake Innovation Forum for International Young Talents, Wuhan, China
- 2017-04 “computations: from atomic clusters to molecular crystals”
The 10th CGCA-WEST Annual Conference, Cologne, Germany
- 2017-03 “computations: from atomic clusters to molecular crystals”
Max Planck Institute for Polymer Research, Germany
- 2016-12 “theoretical studies on the hydrogen activation by frustrated Lewis pairs (FLPs) in solid state”
Max Planck Institute for Chemical Energy Conversion, Germany
- 2016-09 “computations: from atomic clusters to molecular crystals”
Institute of Process Engineering, Chinese Academy of Sciences, China
- 2016-08 “dynamical behavior of boron clusters”
University of Leipzig, Germany
- 2016-06 “computational studies on the hydrogen activation by frustrated Lewis pairs”
RWTH Aachen University, Germany
- 2015-02 “computational studies on the chemistry of boron in gas-phase and solution”
University of Bonn, Germany
- 2014-01 “electronic structure, stability, and reactivity of boron cluster and frustrated Lewis pairs”
University of Amsterdam, the Netherlands