Curriculum Vitae

PERSONAL INFORMATION

Name:	Hui Li
Date of birth:	Dec. 3, 1981
Nationality	Chinese
Language	Chinese, English
Present position:	Associate professor in Institute of Physics, Chinese Academy of Sciences
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EDUCATION

1999 - 2003	B.S. in Department of Intensive Instruction, Nanjing University
2003 - 2008	Ph. D. in Theoretical and Computational Chemistry, Nanjing University Supervisor: Prof. Jing Ma

PROFESSIONAL EXPERIENCES

2003	Teaching Assistant in *Computational Quantum Chemistry*, Nanjing University.
2008	Visiting student in Department of Physics, National University of Singapore.
2008 - 2009	Postdoctoral research fellow in Department of Physics, National University of Singapore. Supervisor: Prof. Andrew T. Wee.
2009 - 2012	Postdoctoral research fellow in Department of Chemistry, University of Nebraska-Lincoln. Supervisor: Prof. Xiao Cheng Zeng.
2012 - Present	Institute Bai-Ren (100-talent) Associate Professor in Institute of Physics, Chinese Academy of Sciences

ACADEMIC HONORS

1999 - 2003	Excellent People' Scholarship from Nanjing University (4 times)
2006	Excellent Graduate Students' Scholarship from Nanjing University
2012	2012 UNL Postdoc Award Honorable Mention

CURRENT RESEARCH INTERESTS

(1) Behaviors of interfacial water/ice and phase transitions

(2) Novel functional materials designing

(3) Structural and dynamical properties of nanostructures/molecules on substrates

(4) Structures, electronics structures and related catalytic properties of metal clusters

(5) Properties of topological insulators

(6) Linear-scaling electronic structure methods

FUNDINGS

(1) Startup funding of IOP (CNY 500,000) 2012-2015

(2) The General Program of NSFC (CNY 760,000) 2014-2018

(3) The Key Program of NSFC (CNY 1,000,000) 2014-2019

(4) The 973 Program (CNY 300,000) 2014-2017

(5) The Program of SKLTP (CNY 200,000) 2013-2014

PUBLICATIONS

Boron and gold clusters

(1) **H. Li**, Y. Pei, X.C. Zeng, **Two-dimensional to three-dimensional structural transition of gold cluster Au-10 during soft landing on TiO2 surface and its effect on CO oxidation,** *J. Chem. Phys.* **2010**, *133*, 134707.

(2) **H. Li**, N. Shao, B. Shang, L.-F. Yuan, J. Yang, X. C. Zeng, **Icosahedral B_{12}-containing core-shell structures of B_{80}**, *Chem. Commun*. **2010**, *46*, 3878.

(3) Y. Pei, N. Shao, **H. Li**, Deen Jiang, and X. C. Zeng, **Hollow Polyhedral Structures in Small Gold-Sulfide Clusters,** *ACS Nano* **2011**, *5*, 1441.

(4) C. Liu, Y. Tan, S. Lin, **H. Li**, X.J. Wu, L. Li, Y. Pei, and X. C. Zeng, **CO Self-Promoting Oxidation on Nanosized Gold Clusters: Triangular Au_3 Active Site and CO Induced O-O Scission**, *J. Am. Chem. Soc.* **2013**, *135*, 2583.

(5) L. Li, Y. Gao, **H. Li,** Y. Zhao, Y. Pei, Z. F. Cheng, X. C. Zeng, **CO Oxidation on TiO2 (110) Supported Subnanometer Gold Clusters: Size and Shape Effects**, *J. Am. Chem. Soc*. **2013**, *135*, 19336.

(6) Y. Zhao, N. S. Khetrapal, **H. Li,** Y. Gao, X. C. Zeng, **Interaction between O_2 and neutral/charged Au_n (n = 1–3) clusters: A comparative study between density-functional theory and coupled cluster calculations**, *Chem. Phys. Lett.* **2014**, *592*, 127.

(7) **H. Li**, L. Li, A. Pedersen, Y Gao, H. Jónsson, X. C. Zeng, **Magic-Number Gold Nanoclusters with diameter 1 to 3.5 nm: Relative Stability and Catalytic Activity for CO Oxidation**, *Nano Letters* **2014**, in press.

Interfacial water/ice

(8) H. X. Zhao*, X. J. Kong*, **H. Li***, Y. C. Jin, L. Long, X. C. Zeng, R. B. Huang, L. S. Zheng, **Transition from one-dimensional water to ferroelectric ice within a supramolecular architecture,** *Proc. Natl. Acad. Sci. USA* **2011**, *108*, 3481. (* co-first author)

(9) **H. Li**, X. C. Zeng, **Wetting and Interfacial Properties of Water Nanodroplets in Contact with Graphene and Monolayer Boron-Nitride Sheets**, *ACS Nano*, **2012**, *6*, 2401.

(10) **H. Li**, X. C. Zeng, **Two Dimensional Epitaxial Water Adlayer on Mica with Graphene Coating: An ab Initio Molecular Dynamics Study,** *J. Chem. Theory Comput.* **2012**, *8*, 3034.

(11) X. Zhou, G. Liu, K. Yamato, Y. Shen, R. Cheng, X. Wei, W. Bai, Y. Gao, **H. Li,** Y. Liu, F. Liu, D. M. Czajkowsky, J. Wang, M. J. Dabney, Z. Cai, J. Hu, F. V. Bright, L. He, X. C. Zeng, Z. Shao, B. Gong, **Self-assembling subnanometer pores with unusual mass-transport properties,** *Nat. Commun.,* **2012**, *3*, 949.

(12) C. Zhu, **H. Li**, Y. Huang, X. C. Zeng, and M. Sheng, **Microscopic Insight into Surface Wetting: Relations between Interfacial Water S tructure and the Underlying Lattice Constant**, *Phys. Rev. Lett.* **2013**, *110*, 126101.

(13) C. Zhu, **H. Li,** X. C. Zeng, E. G. Wang, and S. Meng, **Quantized Water Transport: Ideal Desalination through Graphyne-4 Membrane**, *Sci. Rep.* **2013**, *3*, 3163.

(14) Y. Zhao, **H. Li,** and X. C. Zeng, **First-principles molecular dynamics simulation of atmospherically relevant anion solvation in supercooled water droplet**, *J. Am. Chem. Soc.* **2013**, *135*, 15549.

(15) Z. Chen, G. Wang, Z. Xu, **H. Li**, A. Dhotel, X. C. Zeng, B. Chen, J.-M. Saiter, and L. Tan, **Metal-Organic Frameworks Capable of Healing at Low Temperatures**, *Adv. Mater.* **2013**, *25*, 6106.

(16) S. Chen, **H. Li**, P. Cao, and X. C. Zeng, **Understanding Liquid-Solid-Like Behavior of Tetrahydrofuran Adlayers at Room Temperature between Graphene and Mica: A Born-Oppenheimer Molecular Dynamics Study**, *J. Phys. Chem. C* **2013**, *117*, 21894.

(17) C. Q. Zhu, **Hui Li**, and S. Meng. **Transport behavior of water molecules through two-dimensional nanopores,** *J. Chem. Phys.* **2014**, *141*, 18C502.

(18) L. Pan, G. Liu, **H. Li**, S. Meng, L. Han, J. Jie, B. Chen, A. Platero-Prats, W. Lu, X.D. Zou, R. W. Li. **A Resistance-Switchable and Ferroelectric Metal-Organic Framework**, *J. Am. Chem. Soc.* **2014**, in press.

High pressure materials

(19) L. Wang, B. Liu, **H. Li,** W. Yang, Y. Ding, S. V. Sinogeikin, Y. Meng, Z. Liu, X. C. Zeng, W. L. Mao, **Long-Range Ordered Carbon Clusters: A Crystalline Material with Amorphous Building Blocks,** *Science***, 2012**, *337*, 825.

Low dimensional materials

(20) H. Fu, J. Zhang, Z. Jing, **H. Li*,** S. Meng, **Stacking-dependent electronic structure of bilayer silicene**, *Appl. Phys. Lett.* **2014**, *104*, 131904.

(21) L. Chen, **H. Li,** B. J. Feng, Z. J. Ding, J. L. Qiu, P. Cheng, K. H. Wu, S. Meng, **Spontaneous Symmetry Breaking and Dynamic Phase Transition in Monolayer Silicene**, *Phys. Rev. Lett.* **2013**, *110*, 085504.

(22) B. J. Feng, **H. Li,** C.-C. Liu, T. N. Shao, P. Cheng, Y. G. Yao, S. Meng, L. Chen, K. H. Wu, **Observation of Dirac Cone Warping and Chirality Effects in Silicene**, *ACS Nano*, **2013**, *7*, 9049.

(23) W. Wan, **H. Li,** H. Huang, S. L. Wong, L. Lv, Y. L. Gao, A. Wee, **Incorporating isolated molybdenum (Mo) atoms into Bilayer Epitaxial Graphene on 4H-SiC(0001)**, *ACS Nano*, **2014**, *8*, 970.

(24) Y. H. Yu, L. M. She, H. X. Fu, M. Huang, **H. Li***, S. Meng, G. Y. Cao, **Kondo Effect Mediated Topological Protection: Co on Sb(111).** *ACS Nano* **2014**, *8*, 11576.

Molecules on surfaces

(25) L. Chen, **H. Li**, A.T.S. Wee, **Delocalized State between Molecules through a Surface Confined Pseudodihydrogen Bond**, *Phys. Rev. Lett.* **2010**, *105*, 226103.

(26) K.H.L. Zhang, **H. Li**, H. Mao, H. Huang, J. Ma, A.T.S. Wee, W. Chen, **Control of Two-Dimensional Ordering of F16CuPc on Bi/Ag(111): Effect of Interfacial Interactions**, *J. Phys. Chem. C* **2010**, *114*, 11234.

(27) Y.L. Huang, **H. Li**, J. Ma, H. Huang, W. Chen, A.T.S. Wee, **Scanning Tunneling Microscopy Investigation of Self-Assembled CuPc/F16CUPc Binary Superstructures on Graphite**, *Langmuir* **2010**, *26*, 3329.

(28) Y.L. Huang, W. Chen, **H. Li**, J. Ma, J. Pflaum, A.T.S. Wee, **Tunable Two-Dimensional Binary Molecular Networks**, *Small*, **2010**, *6*, 70.

(29) L. Chen, **Hui Li**, A. T. S. Wee, **Nonlocal Chemical Reactivity at Organic-Metal Interfaces**, *ACS Nano* **2009**, *3*, 3684.

(30) L. Chen, **H. Li**, A. T. S. Wee, **One-Dimensional Molecular Chains with Dispersive Electronic States**, *Nano Lett.*, **2009**, *9*, 4292.

(31) W. Chen, **H. Li**, H. Huang, Y. Fu, J. Ma, A. T. S. Wee, **2D Pentacene:PTCDA supramolecular chiral networks on Ag(111),** *J. Am. Chem. Soc.***2008,** *130*, 12285.

Layered Double Hydroxides simulations

(32) **H. Li,** J. Ma, D. G. Evans, T. Zhou, F. Li, X. Duan, **Molecular Dynamics Modeling of the Structures and Binding Energies of α-Nickel Hydroxides and Nickel-Aluminum Layered Double Hydroxides Containing Various Interlayer Guest Anions**, *Chem. Mater.* **2006**, *18*, 4405.

(33) D. Yan, M. Wei, J. Lu, J. Lan, D. G. Evans, X. Duan, **H. Li,** J. Ma, ***In situ* Polymerization of 4-vinyl-benzenesulfonic Anion in Ni-Al-Layered Double Hydroxide and its Molecular Dynamic Simulation,** *J. Phys. Chem. A* **2008**, *112*, 7671.

(34) H. Yan; M, Wei; J. Ma; **H. Li;** X. Duan, **The Criterion for the Construction of Layers in Layered Double Hydroxides: Theoretical Study Based on the Metal-Oxygen Octahedral Coordination Units,** *J. Mol. Struct.(Theochem)* **2008**, *866*, 34.

Linear scaling QM/MM

(35) **H. Li,** W. Li, S. Li, J. Ma, **Fragmentation-based QM/MM Simulations: Length Dependence of Chain Dynamics and Hydrogen Bonding of Polyethylene Oxide and Polyethylene in Aqueous Solutions**, *J. Phys. Chem. B* **2008**, *112*, 7061.

Others

(36) A. Dhôtel, **H. Li**, L. Fernandez-Ballester, L. Delbreilh, B. Youssef, X.C. Zeng, L. Tan, **Supramolecular Nanolayer Reconfiguration after Molecular Intercalation**, *J. Phys. Chem. B*, **2011**, *115*, 10351.

(37) C. Yu, Z. Chen , **H. Li**, J. Turner, X. C. Zeng, Z. Jin, J. Jiang, B. Youssef, L. Tan, **Molecularly Intercalated Nanoflakes: A Supramolecular Composite for Strong Energy Absorption**, *Adv. Mater.* **2010**, *22*, 4457.

(38) Y. S. Ma, **H. Li,** J. J. Wang, S. S. Bao, R. Cao, Y. Z. Li, J. Ma, L. M. Zheng, **Three-Dimensional Lanthanide(III)-Copper(II) Compounds Based on an Unsymmetrical 2-Pyridylphosphonate Ligand: An Experimental and Theoretical Study** *Chem. Eur. J.* **2007**, *13*, 4759.

(39) X. Yang; X. L. Wua; S. H. Li; **H. Li;** T. Qiu; Y. M. Yang; P. K. Chu; G. G. Siu, **Origin of the 370-nm luminescence in Si oxide nanostructures,** *Appl. Phys. L.* **2005**, *86*, 201906.

(40) Z. G. Chen, Z. P. Xu, M. Zhang, Y. Zhou, M. Z. Liu, T, Patten, G. Y. Liu, **H. Li**, X. C. Zeng, L. Tan, **Two-Dimensional Crystallization of Hexagonal Bilayer with Moiré Patterns,** *J. Phys. Chem. B*, **2012**, *116*, 4363.

(41) F. Zhang, W. Ma, Y. Jiao, J.C. Wang, X.Y. Shan, **H. Li**, X.H. Lu, and S. Meng. **Precise Identification and Manipulation of Adsorption Geometry of Donor-π-Acceptor Dye on Nanocrystalline TiO2 Films for Improved Photovoltaics.** *ACS Appl. Mater. Inter.* **2014**, in press.