CURRICULUM VITAE

Liang Yu, Ph. D.

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Working experience:

2/2015 – 2/2017	Postdoctoral researcher (Supervisor: Prof. Frank Abild-Pedersen) SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering, Stanford University, CA, US SLAC National Accelerator Laboratory, Menlo Park, CA, U.S.
2/2014 – 1/2015	Post-doctoral fellow (Supervisor: Prof. Xinhe Bao, Dr. Ping Liu) Department of Chemistry, Brookhaven National Laboratory, NY, US College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, China
11/2012 – 12/2013	Research Associate (Supervisor: Prof. Xinhe Bao) Nano and Interfacial Catalysis Group, State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

Education:

9/2006 – 10/2012	Ph. D. in Physical Chemistry (Supervisor: Prof. Xinhe Bao) Nano and Interfacial Catalysis Group, State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China
During PhD	
3/2010 – 1/2011	Visiting student (Supervisor: Prof. Peijun Hu) School of Chemistry and Chemical Engineering, The Queen's University of Belfast, Belfast, United Kingdom
7/2008 – 2/2010	Visiting student (Supervisor: Prof. Wei-Xue Li) Center for Theoretical and Computational Chemistry, State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China
9/2001 – 7/2005	B.S. in Applied Chemistry College of Chemical Engineering and Materials Science, Shandong Normal University, Jinan, China

Research Experience

My academic backgrounds include physical chemistry, computational chemistry, heterogeneous catalysis, electrochemical catalysis. My research is focused on solving physicochemical problems in heterogeneous catalysis of chemical reactions related to

sustainable energy conversion and storage.

In my Ph.D. work, I studied carbon-based nanostructures for electro-reduction of oxygen on cathode of fuel cell in collaboration with experiment. The studied materials include nitrogen-doped graphene, nano-sized graphene with abundant edge defects, CNT encapsulating metal nanoparticles, and FeN_4 structure embedded in graphene. In these studies, the active center and catalytic reaction mechanisms are investigated using density functional theory calculations to elucidate the nature of carbon catalysis. The key factors that may affect the electrochemical reaction mechanism such as solvent effect, bias effect, charge effect, and coverage effect were also studied.

After Ph.D. graduation, I studied single-site Fe catalyst for direct methane conversion to ethylene in collaboration with experiment. Using DFT calculations, I proposed the structure of active center as single-atom Fe embedded in SiO_2 matrix through two Fe-C bond and one Fe-Si bond. The mechanism of CH_4 activation on the active center was also studied.

In my postdoctoral project in BNL, I studied the effect of Strong Metal Support Interaction in heterogeneous catalysis using reaction system of CO oxidation at the interfacial sites of FeO_x/Au. My current work is mainly focused on developing approaches for scaling transition state energies on the basis of bond order conservation principle. I have developed a simple scheme for deriving TS scaling relation using only very limited input calculations, but with accuracy comparable or better than BEP method. This method introduces a significant reduction in computational cost compared to current linear approaches.

Research Skills:

- Computational chemistry methods based on density functional theory (VASP, Quantum Espresso, Atomic Simulation Environment).
- Thermodynamics and micro-kinetics study of electrochemical/thermochemical reaction processes.
- Research experience in solvent effect, bias effect, charge effect, and electronic field effect in electrochemical reactions.
- Molecular dynamics simulation.
- Rich experiences in studying reaction mechanism, reaction pathways, electronic structure, and structure-activity relation.
- Strong grasp of chemical phenomena.
- Python programming.
- Conduct in-situ X-ray Absorption Spectrum and X-ray Diffraction experiments.
- Experienced skills with Microsoft office suites, work-related software, data-processing software.

Projects I have taken part in and made significant contributions:

- Developing approaches of predicting transition states energies from simple descriptors based on bond order conservation principle.
- Laser-activated ultra-fast reactions (CO hydrogenation) on Ru metal surface under high temperature.
- Confined interface of metal/metal-oxides for catalytic CO oxidation.
- Single-site catalyst (iron embedded in silicon oxide matrix) for direct conversion of methane to ethylene, and benzene.
- Graphene-based materials as electro-catalyst for oxygen reduction reaction on cathode of fuel cells.
- Carbon nanotubes encapsulating metal nanoparticles as electro-catalyst for oxygen reduction reaction on cathode of fuel cells.

Publication List (Sorted by time):

(1) **Yu, L.**; Abild-Pedersen, F. Bond Order Conservation Strategies in Catalysis Applied to the NH3 Decomposition Reaction. *ACS Catalysis* **2017,** *7*, 864-871.

(2) Chen, X.; **Yu, L.** (co-first author); Wang, S.; Deng, D.; Bao, X. Highly active and stable single iron site confined in graphene nanosheets for oxygen reduction reaction. *Nano Energy* **2017,** *32*, 353-358.

(3) **Yu, L.**; Liu, Y.; Yang, F.; Evans, J.; Rodriguez, J. A.; Liu, P. CO oxidation on gold-supported iron oxides: New insights into strong oxide–metal interactions. *The Journal of Physical Chemistry C* **2015,** *119*, 16614-16622.

(4) Ning, Y.; Wei, M.; **Yu, L.**; Yang, F.; Chang, R.; Liu, Z.; Fu, Q.; Bao, X. Nature of Interface Confinement Effect in Oxide/Metal Catalysts. *The Journal of Physical Chemistry C* **2015,** *119*, 27556-27561.

(5) Deng, D.; Chen, X.; **Yu, L.**; Wu, X.; Liu, Q.; Liu, Y.; Yang, H.; Tian, H.; Hu, Y.; Du, P. A single iron site confined in a graphene matrix for the catalytic oxidation of benzene at room temperature. *Science advances* **2015,** *1*, e1500462.

(6) Chen, X.; Xiao, J.; Wang, J.; Deng, D.; Hu, Y.; Zhou, J.; **Yu, L.**; Heine, T.; Pan, X.; Bao, X. Visualizing electronic interactions between iron and carbon by X-ray chemical imaging and spectroscopy. *Chemical Science* **2015,** *6*, 3262-3267.

(7) Li, X.; Pan, X.; **Yu, L.**; Ren, P.; Wu, X.; Sun, L.; Jiao, F.; Bao, X. Silicon carbide-derived carbon nanocomposite as a substitute for mercury in the catalytic hydrochlorination of acetylene. *Nature communications* **2014,** *5*.

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(9) Guo, X.; Fang, G.; Li, G.; Ma, H.; Fan, H.; **Yu, L.**; Ma, C.; Wu, X.; Deng, D.; Wei, M. Direct, nonoxidative conversion of methane to ethylene, aromatics, and hydrogen. *Science* **2014,** *344*, 616-619.

(10) Deng, J.; Ren, P.; Deng, D.; **Yu, L.**; Yang, F.; Bao, X. Highly active and durable non-precious-metal catalysts encapsulated in carbon nanotubes for hydrogen evolution reaction. *Energy & Environmental Science* **2014,** *7*, 1919-1923.

(11) Zhang, F.; Pan, X.; Hu, Y.; **Yu, L.**; Chen, X.; Jiang, P.; Zhang, H.; Deng, S.; Zhang, J.; Bolin, T. B. Tuning the redox activity of encapsulated metal clusters via the metallic and semiconducting character of carbon nanotubes. *Proceedings of the National Academy of Sciences* **2013,** *110*, 14861-14866.

(12) Wang, Z.-j.; Wei, M.; Jin, L.; Ning, Y.; **Yu, L.**; Fu, Q.; Bao, X. Simultaneous N-intercalation and N-doping of epitaxial graphene on 6H-SiC (0001) through thermal reactions with ammonia. *Nano Research* **2013,** *6*, 399-408.

(13) Deng, J.; **Yu, L.** (co-first author); Deng, D.; Chen, X.; Yang, F.; Bao, X. Highly active reduction of oxygen on a FeCo alloy catalyst encapsulated in pod-like carbon nanotubes with fewer walls. *Journal of Materials Chemistry A* **2013,** *1*, 14868-14873.

(14) Deng, D.; **Yu, L.**; Chen, X.; Wang, G.; Jin, L.; Pan, X.; Deng, J.; Sun, G.; Bao, X. Iron encapsulated within pod-like carbon nanotubes for oxygen reduction reaction. *Angewandte Chemie International Edition* **2013,** *52*, 371-375.

(15) **Yu, L.**; Li, W.-X.; Pan, X.; Bao, X. In-and out-dependent interactions of iron with carbon nanotubes. *The Journal of Physical Chemistry C* **2012,** *116*, 16461-16466.

(16) Mu, R.; Fu, Q.; Jin, L.; **Yu, L.**; Fang, G.; Tan, D.; Bao, X. Visualizing chemical reactions confined under graphene. *Angewandte Chemie International Edition* **2012,** *51*, 4856-4859.

(17) **Yu, L.**; Pan, X.; Cao, X.; Hu, P.; Bao, X. Oxygen reduction reaction mechanism on nitrogen-doped graphene: A density functional theory study. *Journal of catalysis* **2011,** *282*, 183-190.

(18) Guo, S.; Pan, X.; **Yu, L.**; Bao, X. Dispersion of metal nanoparticles on carbon nanotubes with few surface oxygen functional groups. *Materials Letters* **2011,** *65*, 1522-1524.

(19) Deng, D.; **Yu, L.** (co-first author); Pan, X.; Wang, S.; Chen, X.; Hu, P.; Sun, L.; Bao, X. Size effect of graphene on electrocatalytic activation of oxygen. *Chemical Communications* **2011,** *47*, 10016-10018.

(20) Deng, D.; Pan, X.; **Yu, L.**; Cui, Y.; Jiang, Y.; Qi, J.; Li, W.-X.; Fu, Q.; Ma, X.; Xue, Q. Toward N-doped graphene via solvothermal synthesis. *Chemistry of Materials* **2011,** *23*, 1188-1193.

References:

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