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### **Education and Training**

Undergraduate Institution	Major	Degree & Year
Shanghai JiaoTong University	Physics	B.S. (1985)
Graduate Institution	Major/Area	Degree & Year
Cornell University	Physics	Ph.D. (1991)
Postdoctoral Institution	Area	Inclusive Dates
Cornell University	Physics	1991-1992
National Renewable Energy Lab.	Solid-State Physics	1992-1995

### **Research and Professional Experience**

2013-present	<b>Senior Scientist:</b> Lawrence Berkeley National Laboratory, Berkeley, CA
1999-2012	<b>Staff Scientist:</b> Lawrence Berkeley National Laboratory, Berkeley, CA
1996-1999	<b>Staff Scientist:</b> National Renewable Energy Laboratory, Golden, CO
1995-1996	<b>Staff Scientist:</b> Biosym/Molecular Simulations Inc., San Diego, CA

### **PUBLICATIONS**

1. B. Eren, D. Zhrebetskyy, L.L. Patera, C.H. Wu, L.W. Wang, G.A. Somorjai, M. Salmeron, "Activation of Cu(111) surface by decomposition into nanoclusters driven by CO absorption", **Science** 351, 475 (2016).  
a. <https://d2ufo47lrvsv5s.cloudfront.net/content/351/6272/475>
2. J. Ma, L.W. Wang, "Interplay between plasmon and single-particle excitations in a metal nanocluster", **Nature Comm.** 6, 10107 (2015).  
a. <http://www.nature.com/ncomms/2015/151217/ncomms10107/full/ncomms10107.html>
3. Z. Wang, S.S. Li, L.W. Wang, "An efficient real-time time-dependent DFT method and its applications to ion-2D material collision", **Phys. Rev. Lett.** 114, 063004 (2015).  
a. <http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.114.063004>
4. L.W. Wang, "Full selfconsistent solution of the Dyson equation within GW approximation using a plane wave basis set", **Phys. Rev. B**, 91, 125135 (2015).  
a. <http://journals.aps.org/prb/abstract/10.1103/PhysRevB.91.125135>
5. D. Zhrebetskyy, M. Scheele, Y. Zhang, N. Bronstein, C. Thompson, D. Britt, M. Salmeron, P. Alivisatos, L.W. Wang, "Hydroxylation of the surface of PbS nanocrystals passivated with oleic acid", **Science** 344, 1380 (2014).  
a. <http://www.sciencemag.org/content/344/6190/1380.full>
6. J. Kang, J. Li, S.-S. Li, J.-B. Xia, L.W. Wang, "Electronic structural Moire pattern effects on MoS2/MoSe2 2D heterostructures", **Nano Lett.** 13, 5385 (2013).  
<http://pubs.acs.org/doi/abs/10.1021/nl4030648>
7. L. Shi, L.W. Wang, "Ab initio calculations of deep level carrier nonradiative recombination rates in bulk semiconductors", **Phys. Rev. Lett.** 109, 245501 (2012).  
<http://prl.aps.org/abstract/PRL/v109/i24/e245501>
8. G. Zhang, A. Canning, N. Gronbech-Jensen, S. Derenzo, L.W. Wang, "Shallow impurity level calculations in semiconductors using ab initio method", **Phys. Rev. Lett** 110, 166404 (2013).  
<http://prl.aps.org/abstract/PRL/v110/i16/e166404>
9. S. Dag, S.Z. Wang, L.W. Wang, "Large surface dipole moment in ZnO nanorods", **Nano Lett.** 11, 2348 (2011). <http://pubs.acs.org/doi/abs/10.1021/nl200647e>

10. H. Zheng, J. Baker, T. Miller, B. Sadtler, A. Lindenberg, L.W. Wang, C. Kisielowski, A.P. Alivisatos, "Observation of transient structural transformation dynamics in a single Cu<sub>2</sub>S nanorod by TEM", **Science** 333, 206 (2011).  
<http://www.sciencemag.org/content/333/6039/206.short>

## Synergistic activities

- INCITE project award, DOE, 2007-2009, 2010-2012, 2013-2015.
- R&D 100 award, 2013
- Distinguished oversea reviewer for national science projects, Chinese Academy of Science (2013-2015).
- Honorary Professor, Computer Network Information Center 2012.
- Author of the DOE ASCR Joule software metric code: LS3DF, FY 2010.
- Gordon Bell prize, ACM (2008)
- Fellow of American Physical Society (2007).
- Oversea excellent research team, National Natural Science Foundation of China, 2007.
- Oversea young scientist award, National Natural Science Foundation of China, 2003
- Editorial Board, Journal of theoretical and computational nanoscience, 2004-present,

## SOFTWARE PACKAGES

- PEtot: <http://cmsn.lbl.gov/html/PEtot/PEtot.html> (a planewave DFT code)
- PEScan: <http://cmsn.lbl.gov/html/Escan/DOE-nano/pescan.htm> (a folded spectrum code for nanostructure calculations)
- PEtot\_trans: <http://cmsn.lbl.gov/html/Transport/transport.html> (a quantum transport code based on planewave nonlocal pseudopotential Hamiltonian)

## GRADUATE AND POSTDOC ADVISORS AND ADVISEES

*Graduate Advisor:* Prof. Michal Teter, Cornell University

*Postdoctoral Advisor:* Prof. Alex Zunger, University of Colorado

*Graduate Advisee:* Dr. Gaigong Zhang, University of California, Davis; Mr. Chris Barrett, University of California, Berkeley; Dr. Xiangwei Jiang, Semiconductor Institute, CAS

*Postdoctoral Advisee:* Dr. Nenad Vukmirovic, Lawrence Berkeley National Lab; Dr. Shuzhi Wang, Lawrence Berkeley National Lab; Dr. Sefa Dag, Lawrence Berkeley National Lab; Dr. Shiyu Chen, Lawrence Berkeley National Lab; Dr. Danylo Zhrebetskyy, Lawrence Berkeley National Lab; Dr. Kartick Tarafder, Lawrence Berkeley National Lab; Dr. Jie Ma, Lawrence Berkeley National Lab

## Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers

### • Collaborators, past 48 months:

Sefa Dag (Washington University), Aran Garcia-Lekue (Donostia International Physics Center, Spain), Shuzhi Wang (Google Inc.), Ying Luo (Beijing Normal University), Byounghak Lee (Texas State Univ.), Liberato Manna (Istituto Italiano di Tecnologia, Genova), Gabor Somorjai (UC Berkeley), Nenad Vukmirovic (Institute of Physics, Belgrade), Juan Meza (UC Merced), Zhaojun Bai (UC Davis), Suhuai Wei (National Renewable Energy Laboratory), Jianbai Xia (Semiconductor Institute, Beijing, CAS), Jingbo Li (Semiconductor Institute, Beijing, CAS), Shushen Li (Semiconductor Institute, Beijing, CAS), Xiangwei Jiang (Semiconductor Institute, Beijing, CAS), Jean Frechet (UC Berkeley), Yong Zhang

(Univ. North Carolina), Paul Alivisatos (UC Berkeley), Haiping Cheng (Univ. Florida, Miami), Shiyou Chen (Eastern Normal University, Shanghai), Lin Shi (Nanoscience Institute in Suzhou, China), Xingao Gong (Fudan University), Niel Gronbech-Jensen (UC Davis), Emily Carter (Princeton Univ.), Long Wang (Supercomputer Center of CAS, Beijing), Weigua Gao (Fudan University), Danylo Zherebetskyy (LBNL), Nate Lewis (Caltech), Harry Atwater (Caltech.)

