

WEI-QIAO DENG

Director of Active Organic Technology

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Professional Preparation

Lanzhou University, China, Chemistry, B.S., 1994.

Chinese Academy of Science, China, Physical Chemistry, M.S. 1997.

California Institute of Technology, Chemistry, Ph.D. 2004.

California Institute of Technology, Postdoctoral Scholar, 2004-present

University of California, Riverside, Visiting Postdoc, 11/2004-5/2005

Professional Appointments

2005-present *Director of Active Organic Technologies*, Materials and Process Simulation Center, California Institute of Technology.

1997-1998 *Research Assistant*, Dalian Institute of Chemical Physics, P.R. China.

Closely Related Publications:

1. Deng, W.Q.; Flood, A.H.; Stoddart, J.F.; and Goddard, W. A. "An Electrochemical Color-Switchable RGB Dye: Tristable [2]Catenane" *J. Am. Chem. Soc.* 127, 15994-15995, 2005
2. Deng, W.Q.; Muller, R.P.; and Goddard, W.A.; "Mechanism of the Stoddart-Heath bistable rotaxane molecular switch," *J. Am. Chem. Soc.*, 126: 13562-13563, 2004.
3. Deng WQ, Xu X, Goddard WA "A two-stage mechanism of bimetallic catalyzed growth of single-walled carbon nanotubes" *Nano Letters* 4, 2331-2335, 2004.
4. Deng, W.Q.; and Goddard, W.A.; "Predictions of hole mobilities in oligoacene organic semiconductors from quantum mechanical calculations," *J. Phys. Chem. B*, 108: 8614-8621, 2004.
5. Flood AH, Ramirez RJA, Deng WQ, Muller RP, Goddard WA, Stoddart JF "Meccano on the nanoscale - A blueprint for making some of the world's tiniest machines" *Australian J. Chem.* 57, 301-322, 2004.

Other Significant Publications:

1. Deng WQ, Xu X, Goddard WA "New alkali doped pillared carbon materials designed to achieve practical reversible hydrogen storage for transportation" *Phys. Rev. Lett.* 92, 166103, 2004.
2. Deng, W.Q.; Molinero, V.; and Goddard, W.A.; "Fluorinated imidazoles as proton carriers for water-free fuel cell membranes," *J. Am. Chem. Soc.* 126: 15644-15645, 2004.
3. Cheung S, Deng WQ, van Duin ACT, Goddard WA "ReaxFF(MgH) reactive force field for magnesium hydride systems" *J. Phys. Chem. A* 109, 851-859, 2005.
4. Che JW, Cagin T, Deng WQ, Goddard WA "Thermal conductivity of diamond and related materials from molecular dynamics simulations" *J. Chem. Phys.* 113, 6888-6900, 2000.
5. Nielson KD, van Duin ACT, Oxgaard J, Deng WQ, Goddard WA "Development of the ReaxFF reactive force field for describing transition metal catalyzed reactions, with application to the initial stages of the catalytic formation of carbon nanotubes" *J. Phys. Chem. A* 109, 493-499, 2005.

Total 19 SCI journal publications: <http://www.wag.caltech.edu/home/weiqiao/publication.html>

Awards and Honors:

Caltech Outstanding Teaching Assistant Award (2002)

Current Research Interests:

- Molecular/Nanoelectronic: Alternative electronic materials and device structures for ultimate-CMOS and post-CMOS electronics.
- Hydrogen Economy: Hydrogen storage, production and delivery

Professional Memberships:

American Chemistry Society

Other Professional Activities:

- Invited Lecturer, NSF-ITR: 1st CMDF workshop (Caltech, 2005)
- Invited Speaker, 2nd FNANO conference (Utah, 2005)
- Invited Lecturer, NSF-PASI: 2nd Computational Nanotechnology workshop (Caltech, 2004)

Collaborators other than those cited in the publication list:

James R. Heath	Chemistry, Caltech
Yushan Yan	Chemical Engineering, UC Riverside
Florian Gstrein	Intel Component Research
Jagdishbhai U Patel	Flight Electronic, JPL
Richard Kiehl	Electrical Engineering, U. Minnesota
Keli Han	Theoretical Chemistry, Dalian Institute of Chemical Physics, China
Jijie Zhou	Biomedical Engineering, Nanyang Institute of Technology, Singapore

Graduate and post-graduate advisors

William A. Goddard III (graduate and postgraduate advisor)

Current co-Advisees:

Yuki Matsuda	(graduate student)	Xin Zhang	(graduate student)
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Grant Supports:

1. “*Metallic carbon nanotube interconnects for nano-electronics*” (**Co-PI**) Current
Source of support: Intel Total Award: 430,000\$, Jan. 2005-Jan. 2008.
Person-Months per year committed to the project: Cal, 4.0 months.
2. “*Polymer functionalized zeolite proton exchange membrane (PFZ-PEM) for medium temperature (<200 °C) fuel cell*” (**Project Coordinator**) Current
Source of support: DOE Total Award: 900,000\$, Aug. 2005-Aug.2008
Person-Months per year committed to the project: Cal, 4.0 months.
3. “*The Fundamental Science of Ultra-High Density Logic Circuitry*” Current
Source of support: NSF/Nano Total Award: 120,000\$, Aug. 2005-Aug.2008
Person-Months per year committed to the project: Cal, 1.0 months.
4. “*Multi-scale approaches to molecular electronics*” Current
Source of support: MARCO-FENA Total Award: 450,000\$, Dec. 2005-Dec.2008
Person-Months per year committed to the project: Cal, 3.0 months.
6. “*Rational Design and Fundamental Science of Bioanalytical Sensing Elements Based on Carbon Nanotube Arrays for Lab-on-a-Chip*” (**Co-PI**) Pending
Source of support: NSF/MWN Total Award: 300,000\$, Jan. 2006 - Jan.2009
7. “*Active Nanostructure for Nucleic Directed Synthesis of Organic Functional Polymers*” (**Co-PI**) Pending
Source of support: NSF/NIRT Total Award: 1,600,000\$, May 2006 - May 2010