Steven H. Overbury

Distinguished Research Staff
Chemical Functionality Group
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Education

University of New Mexico, Albuquerque	Mathematics	B.S., *Cum Laude*, 1972
University of New Mexico, Albuquerque	Chemistry	B.S., *Magna cum Laude*, 1972
University of California, Berkeley	Physical Chemistry	Ph.D., 1976

Research Interests

Surface Chemistry and Catalysis; structure-function relations in catalysis by Au, cerium oxide and carbon; metal support interactions in catalysis; surface chemistry of oxygenates; electron-proton reactions at electrochemical interfaces, effect of adsorbed cations on O_2 evolution reaction; mesoporous materials; emission control catalysis; *operando* spectroscopy of model catalysts; soft x-ray photoemission for analysis of surface chemisorbates; x-ray absorption for analysis of redox processes in catalysts

Professional Experience:

2006–p	Senior R&D Staff /Catalysis Theme Leader (2006-2011), Chemical Functionality Group, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory (ORNL)
1985–p	Group Leader, Surface Chemistry and Catalysis Group, Chemical Sciences Division, ORNL
2009–p	Leader for Thrust 3, FIRST Energy Frontier Research Center, ORNL
1994–1995	Section Head (Acting), Materials Chemistry, Chemical Sciences Division, ORNL

Professional and Synergistic Activities:

2011	Director, Southeastern Catalysis Society
2010	Co-Organizer, Neutrons for Catalysis: A Workshop on Neutron Scattering Techniques for Studies in Catalysis, ORNL, Sept. 16-17, 2010
2009	Co-Organizer, Catalysis for Fuel Chemistry Symposium, ACS 237th National Meeting, Salt Lake City, Utah, Mar. 22-26, 2010
2009–p	Editorial Board, *Catalysis Letters, Catalysis Communications, Topic in Catalysis*
2009–p	Officer, Southeastern Catalysis Society
2006–2007	Participant, DOE Basic Research Needs Workshop in Combustion, 2006; in Catalysis, 2007
2006	Catalysis Committee, GOLD 2006 International Conference, Limerick, Ireland, Sept. 3-6, 2006
2006–2011	External Advisory Committee, Catalysis and Energy Processes Institute, Northwestern University, Chicago, Illinois
2003	Organizer, National Laboratory Catalysis Conference, Oak Ridge, TN
2002	Workshop Leader, RFA for Nanostructured Materials for Ultra-Selective Catalysis Workshop, Center for Nanophase Materials Sciences, ORNL
2001	Lead PI, Successful NSET Proposal "Nanocatalysis: Synthesis, Properties and Mechanisms,"
1999	Personnel Exchange, Phillips Petroleum Research Lab
1989–1990	Member, ORNL Seed Money Committee
1988	Program Co-Chair, 35th International AVS Symposium & Exhibition, Lakewood, Colorado

Memberships, *American Chemical Society, Tennessee Valley Chapter of American Vacuum Society*

Honors and Awards:

2002	Battelle S&T Challenges Award
1992; 1989	Martin Marietta Energy System (MMES) Publication Award
1987	MMES Technical Achievement Award

Selected Peer-Reviewed Publications *(>100 publications in refereed journals and books) Select List follows CV.*

Collaborators (Last 4 Years; Outside ORNL):
W. Dmowski (Univ. of TN-Knoxville); T. Egami (Univ. of TN-Knoxville); A. Egbebi (Louisiana State Univ.); B. Eichhorn (Univ. of Maryland); S. H. Sun (Brown Univ.); J. J. Spivey (Louisiana State Univ.); M. Flytzani-Stephanopoulos (Tufts Univ.); V. Guliants (Univ. of Cincinnati); R. J. Harrison (Univ. of TN-Knoxville); B. Jang (Texas A&M); S. Pantelides (Vanderbilt Univ.); S. Rashkeev (Idaho National Laboratory); C. S. Song (Pennsylvania State Univ.)

Graduate and Postdoctoral Advisors:
Graduate Advisor: Prof. Gabor Somorjai, University of California-Berkeley

Postdoctoral Scholars Advised (current locations):
Daniela dos Anjos (ORNL); J. Chris Bauer (ORNL); Florencia Calaza (ORNL); Byong-Ku Chang (Chevron Research); Alex Chen (BNL/NSLS); Jason Clark (SudChemie); Wujun Fu (ORNL); Wesley Gordon (Virginia Tech); Meijun Li (ORNL); Zhen Ma (Fudan); Sanjay Senanayake (Brookhaven National Lab/NSLS); Hong Xie (Northwestern Univ.); Lijun Xu (Virginia); Jing Zhou (Univ. of Wyoming)

PUBLICATIONS

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Peer-Reviewed Publications (>100 publications in refereed journals and books)

Z. L. Wu, M. J. Li, and S. H. Overbury, "On the Structure Dependence of CO Oxidation over CeO_2 Nanocrystals with Well-Defined Surface Planes," *Journal of Catalysis* **285**(1), 61-73 (2012).

X. X. Wang, X. L. Ma, V. Schwartz, J. C. Clark, S. H. Overbury, S. Q. Zhao, X. C. Xu, and C. S. Song, "A Solid Molecular Basket Sorbent for CO_2 Capture from Gas Streams with Low CO_2 Concentration under Ambient Conditions," *Physical Chemistry Chemical Physics* **14**(4), 1485-1492 (2012).

S. H. Chai, J. Y. Howe, X. Q. Wang, M. Kidder, V. Schwartz, M. L. Golden, S. H. Overbury, S. Dai, and D. E. Jiang, "Graphitic Mesoporous Carbon as a Support of Promoted Rh Catalysts for Hydrogenation of Carbon Monoxide to Ethanol," *Carbon* **50**(4), 1574-1582 (2012).

Z. L. Wu, A. J. Rondinone, I. N. Ivanov, and S. H. Overbury, "Structure of Vanadium Oxide Supported on Ceria by Multiwavelength Raman Spectroscopy," *Journal of Physical Chemistry C* **115**(51), 25368-25378 (2011).

Z. L. Wu, S. Dai, and S. H. Overbury, "Reply to Comment on "Multiwavelength Raman Spectroscopic Study of Silica-Supported Vanadium Oxide Catalysts," *Journal of Physical Chemistry C* **115**(21), 10925-10928 (2011).

V. Schwartz, H. Xie, H. M. Meyer, S. H. Overbury, and C. D. Liang, "Oxidative Dehydrogenation of Isobutane on Phosphorous-Modified Graphitic Mesoporous Carbon," *Carbon* **49**(2), 659-668 (2011).

V. Schwartz, A. Campos, A. Egbebi, J. J. Spivey, and S. H. Overbury, "EXAFS and FT-IR Characterization of Mn and Li Promoted Titania-Supported Rh Catalysts for CO Hydrogenation," *ACS Catalysis* **1**(10), 1298-1306 (2011).

M. J. Li, Z. L. Wu, and S. H. Overbury, "CO Oxidation on Phosphate-Supported Au Catalysts: Effect of Support Reducibility on Surface Reactions," *Journal of Catalysis* **278**(1), 133-142 (2011).

D. E. Jiang, S. H. Overbury, and S. Dai, "Interaction of Gold Clusters with a Hydroxylated Surface," *Journal of Physical Chemistry Letters* **2**(10), 1211-1215 (2011).

W. J. Fu, J. Kiggans, S. H. Overbury, V. Schwartz, and C. D. Liang, "Low-Temperature Exfoliation of Multilayer-Graphene Material from $FeCl_3$ and CH_3NO_2 Co-Intercalated Graphite Compound," *Chemical Communications* **47**(18), 5265-5267 (2011).

F. C. Calaza, T. L. Chen, D. R. Mullins, and S. H. Overbury, "Structure and Reactivity of Alkyl Ethers Adsorbed on CeO_2(111) Model Catalysts," *Topics in Catalysis* **54**(1-4), 56-69 (2011).

J. C. Bauer, D. Mullins, M. J. Li, Z. L. Wu, E. A. Payzant, S. H. Overbury, and S. Dai, "Synthesis of Silica Supported AuCu Nanoparticle Catalysts and the Effects of Pretreatment Conditions for the CO Oxidation Reaction," *Physical Chemistry Chemical Physics* **13**(7), 2571-2581 (2011).

Z. L. Wu, M. J. Li, J. Howe, H. M. Meyer, and S. H. Overbury, "Probing Defect Sites on CeO_2 Nanocrystals with Well-Defined Surface Planes by Raman Spectroscopy and O_2 Adsorption," *Langmuir* **26**(21), 16595-16606 (2010).

Z. L. Wu, S. Dai, and S. H. Overbury, "Multiwavelength Raman Spectroscopic Study of Silica-Supported Vanadium Oxide Catalysts," *Journal of Physical Chemistry C* **114**(1), 412-422 (2010).

S. N. Rashkeev, S. Dai, and S. H. Overbury, "Modification of Au/TiO_2 Nanosystems by SiO_2 Monolayers: Toward the Control of the Catalyst Activity and Stability," *Journal of Physical Chemistry C* **114**(7), 2996-3002 (2010).

A. Egbebi, V. Schwartz, S. H. Overbury, and J. J. Spivey, "Effect of Li Promoter on Titania-Supported Rh Catalyst for Ethanol Formation from CO Hydrogenation," *Catalysis Today* **149**(1-2), 91-97 (2010).

W. Dmowski, H. F. Yin, S. Dai, S. H. Overbury, and T. Egami, "Atomic Structure of Au Nanoparticles on a Silica Support by an X-Ray PDF Study," *Journal of Physical Chemistry C* **114**(15), 6983-6988 (2010).

L. F. Allard, M. Flytzani-Stephanopoulos, and S. H. Overbury, "Behavior of Au Species in Au/Fe_2O_3 Catalysts Characterized by Novel in Situ Heating Techniques and Aberration-Corrected Stem Imaging," *Microscopy and Microanalysis* **16**(4), 375-385 (2010).

B. Jang, M. Helleson, C. Shi, A. Rondinone, V. Schwartz, C. D. Liang, and S. Overbury, "Characterization of Al_2O_3 Supported Nickel Catalysts Derived from RF Non-Thermal Plasma Technology," *Topics in Catalysis* **49**(3-4), 145-152 (2009).

S. H. Zhou, Z. Ma, H. F. Yin, Z. L. Wu, B. Eichhorn, S. H. Overbury, and S. Dai, "Low-Temperature Solution-Phase Synthesis of NiAu Alloy Nanoparticles via Butyllithium Reduction: Influences of Synthesis Details and Application as the Precursor to Active $Au-NiO/SiO_2$ Catalysts through Proper Pretreatment," *Journal of Physical Chemistry C* **113**(14), 5758-5765 (2009).

H. Xie, Z. L. Wu, S. H. Overbury, C. D. Liang, and V. Schwartz, "Investigation of the Selective Sites on Graphitic Carbons for Oxidative Dehydrogenation of Isobutane," *Journal of Catalysis* **267**(2), 158-166 (2009).

Z. L. Wu, S. H. Zhou, H. G. Zhu, S. Dai, and S. H. Overbury, "DRIFTS-QMS Study of Room Temperature CO Oxidation on Au/SiO_2 Catalyst: Nature and Role of Different Au Species," *Journal of Physical Chemistry C* **113**(9), 3726-3734 (2009).

X. X. Wang, V. Schwartz, J. C. Clark, X. L. Ma, S. H. Overbury, X. C. Xu, and C. S. Song, "Infrared Study of CO_2 Sorption over "Molecular Basket" Sorbent Consisting of Polyethylenimine-Modified Mesoporous Molecular Sieve," *Journal of Physical Chemistry C* **113**(17), 7260-7268 (2009).

S. D. Senanayake, W. O. Gordon, S. H. Overbury, and D. R. Mullins, "Adsorption and Reaction of Acetone over CeO_x(111) Thin Films," *Journal of Physical Chemistry C* **113**(15), 6208-6214 (2009).

C. D. Liang, H. Xie, V. Schwartz, J. Howe, S. Dai, and S. H. Overbury, "Open-Cage Fullerene-Like Graphitic Carbons as Catalysts for Oxidative Dehydrogenation of Isobutane (vol 131, pg7735, 2009)," *Journal of the American Chemical Society* **131**(46), 17030-17030 (2009).

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S. H. Zhou, H. F. Yin, V. Schwartz, Z. L. Wu, D. Mullins, B. Eichhorn, S. H. Overbury, and S. Dai, "In Situ Phase Separation of NiAu Alloy Nanoparticles for Preparing Highly Active Au/NiO CO Oxidation Catalysts," *ChemPhysChem* **9**(17), 2475-2479 (2008).

J. Zhou, A. P. Baddorf, D. R. Mullins, and S. H. Overbury, "Growth and Characterization of Rh and Pd Nanoparticles on Oxidized and Reduced CeO_x(111) Thin Films by Scanning Tunneling Microscopy," *Journal of Physical Chemistry C* **112**(25), 9336-9345 (2008).

H. F. Yin, C. Wang, H. G. Zhu, S. H. Overbury, S. H. Sun, and S. Dai, "Colloidal Deposition Synthesis of Supported Gold Nanocatalysts Based on $Au-Fe_3O_4$ Dumbbell Nanoparticles," *Chemical Communications* (36), 4357-4359 (2008).

H. F. Yin, Z. Ma, S. H. Overbury, and S. Dai, "Promotion of $Au(en)_2Cl_3$-Derived Au/fumed SiO_2 by Treatment with $KMnO_4$," *Journal of Physical Chemistry C* **112**(22), 8349-8358 (2008).

W. F. Yan, Z. Ma, S. M. Mahurin, J. Jiao, E. W. Hagaman, S. H. Overbury, and S. Dai, "Novel $Au/TiO_2/Al_2O_3 \cdot xH_2O$ Catalysts for CO Oxidation," *Catalysis Letters* **121**(3-4), 209-218 (2008).

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N. R. Shiju, V. V. Guliants, S. H. Overbury, and A. J. Rondinone, "Toward Environmentally Benign Oxidations: Bulk Mixed Mo-V-(Te-Nb)-O M1 Phase Catalysts for the Selective Ammoxidation of Propane," *ChemSusChem* **1**(6), 519-523 (2008).

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Z. Ma, S. Brown, J. Y. Howe, S. H. Overbury, and S. Dai, "Surface Modification of Au/TiO_2 Catalysts by SiO_2 via Atomic Layer Deposition," *Journal of Physical Chemistry C* **112**(25), 9448-9457 (2008).

A. Beste, D. R. Mullins, S. H. Overbury, and R. J. Harrison, "Adsorption and Dissociation of Methanol on the Fully Oxidized and Partially Reduced (111) Cerium Oxide Surface: Dependence on the Configuration of the Cerium 4f Electrons," *Surface Science* **602**(1), 162-175 (2008).

H. G. Zhu, Z. Ma, S. H. Overbury, and S. Dai, "Rational Design of Gold Catalysts with Enhanced Thermal Stability: Post Modification of Au/TiO_2 by Amorphous SiO_2 Decoration," *Catalysis Letters* **116**(3-4), 128-135 (2007).

H. G. Zhu, Z. Ma, J. C. Clark, Z. W. Pan, S. H. Overbury, and S. Dai, "Low-Temperature CO Oxidation on Au/fumed SiO_2-based Catalysts Prepared from $Au(en)_2Cl_3$ Precursor," *Applied Catalysis A: General* **326**(1), 89-99 (2007).

V. Schwartz, D. R. Mullins, W. F. Yan, H. G. Zhu, S. Dai, and S. H. Overbury, "Structural Investigation of Au Catalysts on TiO_2-SiO_2 Supports: Nature of the Local Structure of Ti and Au Atoms by EXAFS and XANES," *Journal of Physical Chemistry C* **111**(46), 17322-17332 (2007).

S. N. Rashkeev, A. R. Lupini, S. H. Overbury, S. J. Pennycook, and S. T. Pantelides, "Role of the Nanoscale in Catalytic CO Oxidation by Supported Au and Pt Nanostructures," *Physical Review B* **76**(3), 035438-035446 (2007).

Z. Ma, S. H. Overbury, and S. Dai, "$Au/MxOy/TiO_2$ Catalysts for CO Oxidation: Promotional Effect of Main-Group, Transition, and Rare-Earth Metal Oxide Additives," *Journal of Molecular Catalysis A: Chemical* **273**(1-2), 186-197 (2007).

Z. Ma, C. D. Liang, S. H. Overbury, and S. Dai, "Gold Nanoparticles on Electroless-Deposition-Derived MnOx/C: Synthesis, Characterization, and Catalytic CO Oxidation," *Journal of Catalysis* **252**(1), 119-126 (2007).

Z. Ma, S. Brown, S. H. Overbury, and S. Dai, "$Au/PO_4^{3-}/TiO_2$ and $PO_4^{3-}/Au/TiO_2$ Catalysts for CO Oxidation: Effect of Synthesis Details on Catalytic Performance," *Applied Catalysis A: General* **327**(2), 226-237 (2007).

W. Dmowski, T. Egami, K. E. Swider-Lyons, W. F. Yan, S. Dai, and S. H. Overbury, "Local Atomic Structure in Disordered and Nanocrystalline Catalytic Materials," *Zeitschrift Fur Kristallographie* **222**(11), 617-624 (2007).

J. C. Clark, S. Dai, and S. H. Overbury, "Operando Studies of Desorption, Reaction and Carbonate Formation During CO Oxidation by Au/TiO_2 Catalysts," *Catalysis Today* **126**(1-2), 135-142 (2007).

H. G. Zhu, C. D. Liang, W. F. Yan, S. H. Overbury, and S. Dai, "Preparation of Highly Active Silica-Supported Au Catalysts for CO Oxidation by a Solution-Based Technique," *Journal of Physical Chemistry B* **110**(22), 10842-10848 (2006).

J. Zhou, S. Dag, S. D. Senanayake, B. C. Hathorn, S. V. Kalinin, V. Meunier, D. R. Mullins, S. H. Overbury, and A. P. Baddorf, "Adsorption, Desorption, and Dissociation of Benzene on TiO_2(110) and Pd/TiO_2(110): Experimental Characterization and First-Principles Calculations," *Physical Review B* **74**(12), 125318-125329 (2006).

W. F. Yan, S. M. Mahurin, S. H. Overbury, and S. Dai, "Nanoengineering Catalyst Supports via Layer-by-Layer Surface Functionalization," *Topics in Catalysis* **39**(3-4), 199-212 (2006).

W. F. Yan, S. Brown, Z. W. Pan, S. M. Mahurin, S. H. Overbury, and S. Dai, "Ultrastable Gold Nanocatalyst Supported by Nanosized Non-Oxide Substrate," *Angewandte Chemie-International Edition* **45**(22), 3614-3618 (2006).

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H. G. Zhu, Z. W. Pan, E. W. Hagaman, C. D. Liang, S. H. Overbury, and S. Dai, "Facile One-Pot Synthesis of Gold Nanoparticles Stabilized with Bifunctional Amino/Siloxy Ligands," *Journal of Colloid and Interface Science* **287**(1), 360-365 (2005).

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W. F. Yan, S. M. Mahurin, B. Chen, S. H. Overbury, and S. Dai, "Effect of Supporting Surface Layers on Catalytic Activities of Gold Nanoparticles in CO Oxidation," *Journal of Physical Chemistry B* **109**(32), 15489-15496 (2005).

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W. F. Yan, B. Chen, S. M. Mahurin, S. Dai, and S. H. Overbury, "Brookite-Supported Highly Stable Gold Catalytic System for Co Oxidation," *Chemical Communications* (17), 1918-1919 (2004).

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S. H. Overbury, L. Ortiz-Soto, H. G. Zhu, B. Lee, M. D. Amiridis, and S. Dai, "Comparison of Au Catalysts Supported on Mesoporous Titania and Silica: Investigation of Au Particle Size Effects and Metal-Support Interactions," *Catalysis Letters* **95**(3-4), 99-106 (2004).

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E. W. Hagaman, H. G. Zhu, S. H. Overbury, and S. Dai, "C-13 NMR Characterization of the Organic Constituents in Ligand-Modified Hexagonal Mesoporous Silicas: Media for the Synthesis of Small, Uniform-Size Gold Nanoparticles," *Langmuir* **20**(22), 9577-9584 (2004).

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