

Stanford



Simon R Bare

Distinguished Staff Scientist, SLAC National Accelerator Laboratory

Bio

BIO

Appointments

2016-present Distinguished Staff Scientist, SSRL, SLAC National Accelerator Lab

2010–2016 Research Fellow, UOP LLC, Des Plaines, IL

2003–2010 Senior Research & Development Associate, UOP LLC, Des Plaines, IL

1996–2003 Research & Development Associate, UOP LLC, Des Plaines, IL

1986–1996 Staff Scientist, The Dow Chemical Company, Midland, MI

1984–1986 Postdoctoral Research Associate, Materials & Molecular Research Division, Lawrence Berkeley National Laboratory, Berkeley

1982–1984 Postdoctoral Research Associate, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY

Professional Preparation

University of Liverpool, U.K. Chemistry B.Sc. (Honors) 1979

University of Liverpool, U.K. Physical Chemistry Ph.D. 1982

Workshops Organized:

Conference Chair: “Operando-IV: Recent developments and future perspectives in spectroscopy of working catalysts,” April 2012, Brookhaven National Laboratory

Co-Chair: “Advanced x-ray techniques for catalyst characterization”, ACS National Meeting, April 2017.

Publications

PUBLICATIONS

- **Synthesis of Colloidal Pd/Au Dilute Alloy Nanocrystals and Their Potential for Selective Catalytic Oxidations.** *Journal of the American Chemical Society*
Wrasman, C. J., Boubnov, A., Riscoe, A. R., Hoffman, A. S., Bare, S. R., Cargnello, M.
2018
- **Direct observation of the kinetics of gas–solid reactions using in situ kinetic and spectroscopic techniques** *Reaction Chemistry & Engineering*
Hoffman, A. S., Azzam, S., Zhang, K., Xu, Y., Liu, Y., Bare, S. R., Simonetti, D. A.
2018; 3: 668-675
- **Low-Temperature Restructuring of CeO₂-Supported Ru Nanoparticles Determines Selectivity in CO₂ Catalytic Reduction.** *Journal of the American Chemical Society*
Aitbekova, A., Wu, L., Wrasman, C. J., Boubnov, A., Hoffman, A. S., Goodman, E. D., Bare, S. R., Cargnello, M.

2018; 140 (42): 13736–45

- **High-Energy-Resolution X-ray Absorption Spectroscopy for Identification of Reactive Surface Species on Supported Single-Site Iridium Catalysts** *CHEMISTRY-A EUROPEAN JOURNAL*
Hoffman, A. S., Sokaras, D., Zhang, S., Debeve, L. M., Fang, C., Gallo, A., Kroll, T., Dixon, D. A., Bare, S. R., Gates, B. C.
2017; 23 (59): 14760–68
- **Tuning the Selectivity of Single-Site Supported Metal Catalysts with Ionic Liquids** *ACS CATALYSIS*
Babucci, M., Fang, C., Hoffman, A. S., Bare, S. R., Gates, B. C., Uzun, A.
2017; 7 (10): 6969–72
- **Uniform Pt/Pd Bimetallic Nanocrystals Demonstrate Platinum Effect on Palladium Methane Combustion Activity and Stability** *ACS CATALYSIS*
Goodman, E. D., Dai, S., Yang, A., Wrasman, C. J., Gallo, A., Bare, S. R., Hoffman, A. S., Jaramillo, T. F., Graham, G. W., Pan, X., Cargnello, M.
2017; 7 (7): 4372–80
- **Characterization of Coke on a Pt-Re/gamma-Al₂O₃ Re-Forming Catalyst: Experimental and Theoretical Study** *ACS CATALYSIS*
Bare, S. R., Vila, F. D., Charochak, M. E., Prabhakar, S., Bradley, W. J., Jaye, C., Fischer, D. A., Hayashi, S. T., Bradley, S. A., Rehr, J. J.
2017; 7 (2): 1452–61
- **Coke Formation in a Zeolite Crystal During the Methanol-to-Hydrocarbons Reaction as Studied with Atom Probe Tomography**
Schmidt, J. E., Poplawsky, J. D., Mazumder, B., Attila, O., Fu, D., de Winter, D., Meirer, F., Bare, S. R., Weckhuysen, B. M.
WILEY-VCH VERLAG GMBH.2016: 11173–77
- **Transmission and fluorescence X-ray absorption spectroscopy cell/flow reactor for powder samples under vacuum or in reactive atmospheres** *REVIEW OF SCIENTIFIC INSTRUMENTS*
Hoffman, A. S., Debeve, L. M., Bendjeriou-Sedjerari, A., Ouldchikh, S., Bare, S. R., Basset, J., Gates, B. C.
2016; 87 (7): 073108
- **Surface analysis of zeolites: An XPS, variable kinetic energy XPS, and low energy ion scattering study** *SURFACE SCIENCE*
Bare, S. R., Knop-Gericke, A., Teschner, D., Haevacker, M., Blume, R., Rocha, T., Schloegl, R., Chan, A. Y., Blackwell, N., Charochak, M. E., ter Veen, R., Brongersma, H. H.
2016; 648: 376–82
- **Aberration-Corrected Transmission Electron Microscopy and InSitu XAFS Structural Characterization of Pt-/Al₂O₃ Nanoparticles** *CHEMCATCHEM*
Sinkler, W., Sanchez, S. I., Bradley, S. A., Wen, J., Mishra, B., Kelly, S. D., Bare, S. R.
2015; 7 (22): 3779–87
- **Expanding Beyond the Micropore: Active-Site Engineering in Hierarchical Architectures for Beckmann Rearrangement** *ACS Catalysis*
Newland, S. H., Sinkler, W., Mezza, T., Bare, S. R., Carravetta, M., Haies, I. M., Levy, A., Keenan, S., Raja, R.
2015; 5 (11): 6587–93
- **Spectroscopic and Computational Insights on Catalytic Synergy in Bimetallic Aluminophosphate Catalysts** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Potter, M. E., Paterson, A. J., Mishra, B., Kelly, S. D., Bare, S. R., Cora, F., Levy, A. B., Raja, R.
2015; 137 (26): 8534-8540
- **Determining the location and nearest neighbours of aluminium in zeolites with atom probe tomography** *NATURE COMMUNICATIONS*
Perea, D. E., Arslan, I., Liu, J., Ristanovic, Z., Kovarik, L., Arey, B. W., Lercher, J. A., Bare, S. R., Weckhuysen, B. M.
2015; 6
- **Characterization of a Fluidized Catalytic Cracking Catalyst on Ensemble and Individual Particle Level by X-ray Micro- and Nanotomography, Micro-X-ray Fluorescence, and Micro-X-ray Diffraction** *CHEMCATCHEM*
Bare, S. R., Charochak, M. E., Kelly, S. D., Lai, B., Wang, J., Chen-Wiegart, Y.
2014; 6 (5): 1427–37
- **Pressure-Dependent Effect of Hydrogen Adsorption on Structural and Electronic Properties of Pt/gamma-Al₂O₃ Nanoparticles** *CHEMCATCHEM*
Mistry, H., Behafarid, F., Bare, S. R., Roldan Cuenya, B.
2014; 6 (1): 348–52
- **Interplay between nanoscale reactivity and bulk performance of H-ZSM-5 catalysts during the methanol-to-hydrocarbons reaction** *JOURNAL OF CATALYSIS*

Aramburo, L. R., Teketel, S., Svelle, S., Bare, S. R., Arstad, B., Zandbergen, H. W., Olsbye, U., de Groot, F. F., Weckhuysen, B. M.
2013; 307: 185–93

- **Operando Effects on the Structure and Dynamics of PtSn/gamma-Al₂O₃ from Ab Initio Molecular Dynamics and X-ray Absorption Spectra** *JOURNAL OF PHYSICAL CHEMISTRY C*
Vila, F. D., Rehr, J. J., Kelly, S. D., Bares, S. R.
2013; 117 (24): 12446–57
- **EXAFS Model of 2-Dimensional Platinum Clusters**
Kelly, S. D., Charochak, M. E., Blackwell, N., Bare, S. R., Wu, Z. Y.
IOP PUBLISHING LTD.2013
- **Electronic properties and charge transfer phenomena in Pt nanoparticles on gamma-Al₂O₃: size, shape, support, and adsorbate effects** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
Behafarid, F., Ono, L. K., Mostafa, S., Croy, J. R., Shafai, G., Hong, S., Rahman, T. S., Bare, S. R., Roldan Cuenya, B.
2012; 14 (33): 11766–79
- **Controlled one-step synthesis of hierarchically structured macroscopic silica spheres** *MICROPOROUS AND MESOPOROUS MATERIALS*
Scholz, S., Bare, S. R., Kelly, S. D., Lercher, J. A.
2011; 146 (1-3): 18–27
- **Density functional theory study of the effect of subsurface H, C, and Ag on C₂H₂ hydrogenation on Pd(1 1 1)** *CATALYSIS TODAY*
Tiruppathi, P., Low, J. J., Chan, A. Y., Bare, S. R., Meyer, R. J.
2011; 165 (1): 106–11
- **Experimental (XAS, STEM, TPR, and XPS) and Theoretical (DFT) Characterization of Supported Rhenium Catalysts** *JOURNAL OF PHYSICAL CHEMISTRY C*
Bare, S. R., Kelly, S. D., Vila, F. D., Boldingh, E., Karapetrova, E., Kas, J., Mickelson, G. E., Modica, F. S., Yang, N., Rehr, J. J.
2011; 115 (13): 5740–55
- **Simultaneous XAFS measurements of multiple samples** *JOURNAL OF SYNCHROTRON RADIATION*
Ravel, B., Scorzato, C., Siddons, D. P., Kelly, S. D., Bare, S. R.
2010; 17: 380–85
- **Characterizing industrial catalysts using in situ XAFS under identical conditions** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
Bare, S. R., Kelly, S. D., Ravel, B., Greenlay, N., King, L., Mickelson, G. E.
2010; 12 (27): 7702–11