

# Simon Podkolzin

Associate Professor  
**Department of Chemical Engineering and Materials Science**  
**Stevens Institute of Technology**  
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- 1988 - **BS-MS in Chemical Engineering** – State University of Oil & Gas, Moscow, Russia
  - 1991 - **Graduate Diploma** in Intellectual Property – University of London, England, UK
  - 1991-1995 - **Research Engineer** – UOP, Guildford, Surrey, UK and Des Plaines, Illinois
  - 1995-2001 – **PhD in Chemical Engineering** – University of Wisconsin – Madison
  - 2002-2008 - **Senior Research Engineer** – The Dow Chemical Company, Midland, Michigan
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Heterogeneous catalysis at molecular level, kinetic testing, infrared spectroscopy, density functional theory (DFT) calculations with vibrational analyses, kinetic modeling and molecular simulations of surface reactions.

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## Current projects

- Molecular fundamentals of natural gas conversion to liquid chemicals over Mo/ZSM-5.
- Acetylene adsorption and conversion to benzene on Pt-Sn alloys.
- Catalytic gold and silver nanoparticles for direct synthesis of hydrogen peroxide and olefin epoxidation.

## Courses (Chemical Engineering, Materials Science, Nanotechnology)

- CHE-345: Chemical Process Control, Modeling and Simulation.
- CHE-424: Engineering Design VIII.
- NANO-525 (CH, MT, PEP): Techniques of Surface and Nanostructure Characterization.
- CHE-555 (MT, NANO, EN): Catalysis and Characterization of Nanoparticles.
- NANO-600: Applications of Nanoscience and Nanotechnology.
- CHE-620 (MT-603): Chemical Engineering Thermodynamics.

## Synergistic activities

- Chairman: *Catalysis Society of Metropolitan New York* (2011-present).
- Awardee: Travel Award of the *North American Catalysis Society* for presenting at the *International Congress on Catalysis*, Munich, Germany, 2012.
- Chairman: *Applications of Computational Methods to Environmentally Sustainable Solutions*, American Chemical Society (Division of Computers in Chemistry), San Diego, CA, 2012.
- Reviewer: *Journal of Catalysis*, *Journal of Physical Chemistry*, *Chemistry of Materials*, *Catalysis Communications*, *Chemical Engineering Journal*.

**Recent publications and conference proceedings**

1. T. Chen; J.M. Jehng, A. Pal; S.G. Podkolzin and I.E. Wachs; *Identification of oxygen species active in ethylene epoxidation on silver catalysts with Raman spectroscopy and DFT calculations*. International Congress on Catalysis, Munich, Germany, **2012**.
2. X. Yang; J. Gao; S.G. Podkolzin and B.E. Koel; *Modifying selectivity of hydrocarbon conversion reactions by alloying Sn and Pt: benzene formation from acetylene*. American Vacuum Society 59<sup>th</sup> International Symposium, Tampa, FL, **2012**.
3. J. Gao; H. Zhao; X. Yang; B.E. Koel and S.G. Podkolzin; *Experimental spectroscopic and computational DFT studies of the mechanism of acetylene conversion to benzene on Pt-Sn alloys*. American Chemical Society National Meeting, San Diego, CA, **2012**.
4. J. Gao; J.M. Jehng; G. B. Fitzgerald; S.G. Podkolzin and I.E. Wachs; *Identification of catalytic molybdenum nanostructures on ZSM-5 for natural gas processing based on DFT calculation and operando molecular spectroscopy*. American Chemical Society National Meeting, San Diego, CA, **2012**.
5. J. Gao; J.M. Jehng; G. B. Fitzgerald; I.E. Wachs and S.G. Podkolzin; *Identification of Supported Molybdenum Nanostructures for Catalytic Methane Aromatization with Operando Molecular Spectroscopy and DFT Calculations*, Nanotechnology Today Conference, Kona, Hawaii, **2011**.
6. J. Gao; J.M. Jehng; G. B. Fitzgerald; S.G. Podkolzin and I.E. Wachs; *Studies of methane aromatization over Mo/ZSM-5 catalysts with operando molecular spectroscopy and DFT calculations*. European Catalysis Conference EuropaCat X, Glasgow, Scotland, UK, **2011**.
7. J. Gao; E. de Smit; G.B. Fitzgerald; A. Lawal; B. Weckhuysen and S.G. Podkolzin; *Dynamic characterization of Co/TiO<sub>2</sub> Fischer-Tropsch catalysts with infrared spectroscopy and DFT calculations*. 22<sup>nd</sup> North American Catalysis Society Meeting, Detroit, MI, **2011**.
8. J. Gao; H. Zhao; X. Yang; B.E. Koel and S.G. Podkolzin; *Study of acetylene adsorption and reactivity on Pt and Pt-Sn alloys with HREELS, TPD and DFT calculations*. 22<sup>nd</sup> North American Catalysis Society Meeting, Detroit, MI, **2011**.
9. J. Gao; J.M. Jehng; G. B. Fitzgerald; S.G. Podkolzin and I.E. Wachs; *Investigation of methane aromatization over Mo/ZSM-5 catalysts with DFT calculations and operando Molecular spectroscopy*. 22<sup>nd</sup> North American Catalysis Society Meeting, Detroit, MI, **2011**.
10. T. Chen; J.M. Jehng; A. Pal; S.G. Podkolzin and I.E. Wachs; *Identification of catalytic active oxygen species on alumina-supported silver nanoparticles with in situ Raman spectroscopy and DFT calculations*. 22<sup>nd</sup> North American Catalysis Society Meeting, Detroit, MI, **2011**.
11. J.M. Jehng; J. Gao; S.G. Podkolzin and I.E. Wachs; *Investigation of methane conversion to benzene over Mo/ZSM-5 catalysts with operando molecular spectroscopy and DFT calculations*. American Chemical Society National Meeting, Anaheim, CA, **2011**.
12. J. Gao; E. de Smit; B. Weckhuysen and S.G. Podkolzin; *Dynamic characterization of Co/TiO<sub>2</sub> Fischer-Tropsch catalysts with infrared spectroscopy and DFT calculations*. American Chemical Society National Meeting, Anaheim, CA, **2011**.

13. T. Chen; J.M. Jehng; A. Pal; S.G. Podkolzin and I.E. Wachs; *Identification of catalytic active oxygen species on alumina-supported silver nanoparticles with in situ Raman spectroscopy and DFT calculations*. American Chemical Society National Meeting, Anaheim, CA, **2011**.
14. J. Kim; L.A. Welch; A. Olivas; S.G. Podkolzin and B.E. Koel; *Adsorption and Decomposition of Cyclohexanone (C<sub>6</sub>H<sub>10</sub>O) on Pt(111) and the (2 × 2) and ( $\sqrt{3} \times \sqrt{3}$ )R30°-Sn/Pt(111) Surface Alloys*. Langmuir, *26*(21), 16401-16411, **2010**.
15. J. Kim; J. Fu; S.G. Podkolzin and B.E. Koel; *Studies of ethylene oxide adsorption on Pt-Sn alloys with TPD, HREELS, UPS, and DFT calculations*. Journal of Physical Chemistry C, *114*(40), 17238-17247, **2010**.
16. J. Gao; E. de Smit; B. Weckhuysen and S.G. Podkolzin; *Dynamic characterization of surfaces of Co/TiO<sub>2</sub> Fischer-Tropsch catalysts with infrared spectroscopy and DFT calculations*. International Novel Gas Conversion Conference, Lyon, France, **2010**.
17. Y.D. Dai; J.M. Jehng; J. Gao; I.E. Wachs and S.G. Podkolzin; *Investigation of Methane Aromatization over Mo/ZSM-5 Catalysts with Operando Molecular Spectroscopy and DFT Calculations*. International Novel Gas Conversion Conference, Lyon, France, **2010**.
18. D.A. Hickman; M.E. Jones; Z.R. Jovanovic; M.M. Olken; S.G. Podkolzin; E.E. Stangland and R.K. Thompson; *Reactor Scale-up for Fluidized Bed Conversion of Ethane to Vinyl Chloride*. Industrial & Engineering Chemistry Research, *49*(21), 10674-10681, **2010**.
19. J.E. Molinari; I.E. Wachs and S.G. Podkolzin; *Existence of Vanadium Umbrella Structure in Biocatalyst Systems Only*. American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT, **2010**.
20. I.E. Wachs; J.M. Jehng and S.G. Podkolzin, S.G.; *Investigation of methane aromatization over Mo/ZSM-5 catalysts with operando spectroscopy and DFT calculations*. American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT, **2010**.
21. Y.D. Dai; J.M. Jehng; S.G. Podkolzin; B. Modak and I.E. Wachs; *Investigation of methane aromatization over Mo/ZSM-5 catalysts with operando spectroscopy and DFT calculations*. American Chemical Society National Meeting, Boston, MA, **2010**.
22. Podkolzin and T.A. Nijhuis; *Spectroscopic and DFT computational study of TiO<sub>2</sub> catalyst deactivation in propylene selective oxidation*. American Chemical Society National Meeting, Washington, DC, **2009**.
23. A.W.A.M. van der Heijden; S.G. Podkolzin; M.E. Jones; J.H. Bitter and B.M. Weckhuysen; *Catalytic hydrogen-chlorine exchange between chlorinated hydrocarbons under oxygen-free conditions*. Angewandte Chemie - International Edition, *47*(27), 5002-5004, **2008**.
24. S.G. Podkolzin; E.E. Stangland; M.E. Jones; E. Peringer and Lercher, J.A.; *Methyl chloride production from methane over lanthanum-based catalysts*. Journal of the American Chemical Society, *129*(9), 2569-2576, **2007**.