Stanford

Shyama Mandal

Postdoctoral Scholar, Photon Science, SLAC

Bio

STANFORD ADVISORS

- Frank Abild-Pedersen, Postdoctoral Research Mentor
- Thomas Jaramillo, Postdoctoral Faculty Sponsor

Publications

PUBLICATIONS

- **Enhancing CO Oxidation Rate via Electronic Tuning of CO Binding on Bimetallic Nanoparticle Catalysts.** *Journal of the American Chemical Society*
  Chung, P. H., Xie, S., Li, X., Mandal, S. C., Zhang, Z., Oh, J., Liu, F., Abild-Pedersen, F., Sánchez-Carrera, R. S., Lizandara-Pueyo, C., Li, Y., Cargnello, M.
  2026
- **Tailored Rh-Al₂O₃-ZrO₂ Interfaces: Insights into Rh Aluminate Formation and Enhanced Stability** *CHEMISTRY OF MATERIALS*
  Liccardo, G., Nhan, B. T., Chung, P., Hutton, D., D'Acunto, G., Mandal, S. C., Smith, J., Richardson, S., Chi, M., Abild-Pedersen, F., Bent, S. F., Cargnello, M.
  2026
- **Dependence of catalytic properties of strongly supported platinum clusters with atom counts.** *Science (New York, N.Y.)*
  Song, C. K., Jung, J., Mandal, S. C., Kang, S., Kim, T. Y., Kim, C., Jang, G., Kim, H., Kim, Y., Lee, K. R., Kim, J. S., Chen, J., Kim, et al
  2026; 392 (6801): 958-965
- **Effect of Oxide Chemistry on Pt Redistribution and Site Exposure in ALD-Coated Catalysts** *ACS CATALYSIS*
  Nhan, B. T., Mandal, S. C., Smith, J., Liccardo, G., Richardson, S., Abild-Pedersen, F., Chi, M., Cargnello, M., Bent, S. F.
  2026
- **A physics informed model for the prediction of surface energies and the shape of metal particles.** *iScience*
  Mandal, S. C., Abild-Pedersen, F.
  2026; 29 (1): 114430
- **A physics informed model for the prediction of surface energies and the shape of metal particles** *ISCIENCE*
  Mandal, S., Abild-Pedersen, F.
  2026; 29 (1)
- **Toward Instant Prediction of Metal Adatom Diffusion Barriers for Understanding of Sintering and Catalyst Durability** *JOURNAL OF PHYSICAL CHEMISTRY C*
  Deo, S., Mandal, S., Saini, S., Abild-Pedersen, F.
  2025
- **Crossing the Oxo-Peroxo Wall for Selective Electrochemical Epoxidation.** *Advanced science (Weinheim, Baden-Wurttemberg, Germany)*
  Basera, P., Mandal, S. C., Abild-Pedersen, F., Bajdich, M.
  2025: e17229
- **Metal-Independent Correlations for Site-Specific Binding Energies of Relevant Catalytic Intermediates.** *JACS Au*
  Mandal, S. C., Abild-Pedersen, F.

2024; 4 (12): 4790-4798

- **Metal-Independent Correlations for Site-Specific Binding Energies of Relevant Catalytic Intermediates** *JACS AU*
  Mandal, S., Abild-Pedersen, F.
  2024
- **Dehydrogenative Coupling for Synthesis of Quinazolin-4(3H)-ones via Tandem Reaction using Ruthenium(II)-Phenyl-Azo-Naphthaldoxime:AnExperimental and Theoretical Investigation.** *Chemistry, an Asian journal*
  Halder, S., Naskar, S., Jana, D., Kanrar, G., Mandal, S. C., Roy, S., Bharadwaj, N., Pramanik, K., Ganguly, S.
  2024: e202401278
- **Unveiling the Stability of Encapsulated Pt Catalysts Using Nanocrystals and Atomic Layer Deposition.** *Journal of the American Chemical Society*
  Liccardo, G., Cendejas, M. C., Mandal, S. C., Stone, M. L., Porter, S., Nhan, B. T., Kumar, A., Smith, J., Plessow, P. N., Cegelski, L., Osio-Norgaard, J., Abild-Pedersen, F., Chi, et al
  2024
- **Sintering Mechanism of Pt/Al₂O₃ in Complex Emission Gases Elucidated via In Situ Environmental STEM** *ACS MATERIALS LETTERS*
  Smith, J., Liccardo, G., Cendejas, M. C., Stone, M., Mandal, S., Abild-Pedersen, F., Cargnello, M., Chi, M.
  2024
- **Machine learning-based screening of Mn-PNP catalysts for the CO₂ reduction reaction using a region-wise ligand-encoded feature matrix** *ENERGY ADVANCES*
  Das, A., Roy, D., Mandal, S., Pathak, B.
  2024
- **Unravelling CO2 Reduction Reaction Intermediates on High Entropy Alloy Catalysts: An Interpretable Machine Learning Approach To Establish Scaling Relations.** *Chemistry (Weinheim an der Bergstrasse, Germany)*
  Roy, D., Charan Mandal, S., Das, A., Pathak, B.
  2023: e202302679
- **Classification of Adsorbed Hydrocarbons Based on Bonding Configurations of the Adsorbates and Surface Site Stabilities** *ACS CATALYSIS*
  Mandal, S., Abild-Pedersen, F.
  2023: 13663-13671
- **Organic additive for the selective C-2-product formation on Cu(100): a density functional theory mechanistic study** *CATALYSIS SCIENCE & TECHNOLOGY*
  Das, A., Mandal, S., Pathak, B.
  2023
- **Energy level alignments between organic and inorganic layers in 2D layered perovskites: conjugation vs. substituent.** *Nanoscale*
  Mahal, E., Mandal, S. C., Roy, D., Pathak, B.
  2023
- **Subsurface Li Monolayer on Cu(111) Surfaces for Upgrading Ethanol to n-Butanol: A Computational Study** *ACS APPLIED NANO MATERIALS*
  Pathak, B., Tiwari, M., Mandal, S., Das, A.
  2023
- **Ga and Zn Atom-Doped CuAl2O4(111) Surface-Catalyzed CO2 Conversion to Dimethyl Ether: Importance of Acidic Sites** *JOURNAL OF PHYSICAL CHEMISTRY C*
  Pathak, B., Das, A., Mandal, S., Das, S.
  2022; 126 (51): 21628-21637
- **Antibiotic-triggered reversible luminescence switching in amine-grafted mixed-linker MOF: exceptional turn-on and ultrafast nanomolar detection of sulfadiazine and adenosine monophosphate with molecular keypad lock functionality** *JOURNAL OF MATERIALS CHEMISTRY A*
  Goswami, R., Mandal, S., Seal, N., Pathak, B., Neogi, S.
  2019; 7 (33): 19471-19484

- **Guest-Induced Ultrasensitive Detection of Multiple Toxic Organics and Fe³⁺ Ions in a Strategically Designed and Regenerative Smart Fluorescent Metal-Organic Framework** *ACS APPLIED MATERIALS & INTERFACES*
  Goswami, R., Mandal, S., Pathak, B., Neogi, S.
  2019; 11 (9): 9042-9053