



Frank Abild-Pedersen

Senior Scientist, SLAC National Accelerator Laboratory

Bio

BIO

Dr. Abild-Pedersen is the co-director of SUNCAT Center for Interface Science and Catalysis. He is leading a research team that focuses on developing an understanding of the factors determining the catalytic properties at the interface between gas/solvent and solid surfaces and to apply these insights to processes and catalysts of importance for energy transformations and for sustainable chemical production. His research takes advantage of computer facilities at SLAC and Stanford to gain the necessary understanding and to link these simulations to experiments where new catalyst synthesis methods are developed, and the catalyst materials are characterized both in terms of performance (activity, selectivity, durability, etc.) and in terms of geometrical and electronic structure. The underlying philosophy of his research is that by having a fundamental understanding of the way surfaces catalyze a chemical reaction we can make a quantum leap in our ability to make predictions for new catalysts and processes. This requires the development of a theory of heterogeneous catalysis, including electrocatalysis, based on computational and experimental results.

Dr Abild-Pedersen has extensive experience with simulations and modeling of chemical reactions. His work began with the derivation of energy correlations in catalysis that have helped speed up screening for active, selective and stable catalysts for energy conversion as a graduate student working with Professor Jens K. Nørskov at the Technical University of Denmark. He moved to SLAC in 2010 as a staff scientist and helped build up SUNCAT and define research directions in the field of heterogeneous catalysis.

EDUCATION AND CERTIFICATIONS

- PhD, Technical University of Denmark , Physics (2005)

Publications

PUBLICATIONS

- **Oxidizing Role of Cu Cocatalysts in Unassisted Photocatalytic CO₂Reduction Using p-GaN/Al₂O₃/Au/Cu Heterostructures.** *ACS nano*
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2024

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- **Interpretable design of Ir-free trimetallic electrocatalysts for ammonia oxidation with graph neural networks (vol 14, 792, 2023)** *NATURE COMMUNICATIONS*
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- **Classification of Adsorbed Hydrocarbons Based on Bonding Configurations of the Adsorbates and Surface Site Stabilities** *ACS CATALYSIS*
Mandal, S., Abild-Pedersen, F.
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- **A Comparative Study of Electrical Double Layer Effects for CO Reduction Reaction Kinetics** *JOURNAL OF PHYSICAL CHEMISTRY C*
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 - **Unraveling Electronic Trends in O* and OH* Surface Adsorption in the MO₂ Transition-Metal Oxide Series** *JOURNAL OF PHYSICAL CHEMISTRY C*
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- **Dynamics and Hysteresis of Hydrogen Intercalation and Deintercalation in Palladium Electrodes: A Multimodal In Situ X-ray Diffraction, Coulometry, and Computational Study** *CHEMISTRY OF MATERIALS*
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