



## Frank Abild-Pedersen

Senior Scientist, SLAC National Accelerator Laboratory

### Bio

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#### 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

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#### PUBLICATIONS

- **Electronic structure factors and the importance of adsorbate effects in chemisorption on surface alloys** *NPJ COMPUTATIONAL MATERIALS*  
Saini, S., Halldin Stenlid, J., Abild-Pedersen, F.  
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- **Screening binary alloys for electrochemical CO<sub>2</sub> reduction towards multi-carbon products** *JOURNAL OF MATERIALS CHEMISTRY A*  
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- **Unraveling Electronic Trends in O\* and OH\* Surface Adsorption in the MO<sub>2</sub> Transition-Metal Oxide Series** *JOURNAL OF PHYSICAL CHEMISTRY C*  
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- **Enhancing the connection between computation and experiments in electrocatalysis** *NATURE CATALYSIS*

- Resasco, J., Abild-Pedersen, F., Hahn, C., Bao, Z., Koper, M. M., Jaramillo, T. F.  
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- **Catalytic Performance and Near-Surface X-ray Characterization of Titanium Hydride Electrodes for the Electrochemical Nitrate Reduction Reaction.** *Journal of the American Chemical Society*  
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  - **Colloidal Platinum-Copper Nanocrystal Alloy Catalysts Surpass Platinum in Low-Temperature Propene Combustion.** *Journal of the American Chemical Society*  
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2022
  - **Exploring Trends on Coupling Mechanisms toward C-3 Product Formation in CO(2)R** *JOURNAL OF PHYSICAL CHEMISTRY C*  
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  - **Modeling Potential-Dependent Electrochemical Activation Barriers: Revisiting the Alkaline Hydrogen Evolution Reaction.** *Journal of the American Chemical Society*  
Li, J., Stenlid, J. H., Ludwig, T., Lamoureux, P. S., Abild-Pedersen, F.  
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  - **Combining artificial intelligence and physics-based modeling to directly assess atomic site stabilities: from sub-nanometer clusters to extended surfaces.** *Physical chemistry chemical physics : PCCP*  
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  - **Guiding the Catalytic Properties of Copper for Electrochemical CO<sub>2</sub> Reduction by Metal Atom Decoration.** *ACS applied materials & interfaces*  
Nishimura, Y. F., Peng, H. J., Nitopi, S., Bajdich, M., Wang, L., Morales-Guio, C. G., Abild-Pedersen, F., Jaramillo, T. F., Hahn, C.  
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- **Revealing the Synergy between Oxide and Alloy Phases on the Performance of Bimetallic In-Pd Catalysts for CO<sub>2</sub> Hydrogenation to Methanol** *ACS CATALYSIS*  
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