

Stanford



Frank Abild-Pedersen

Senior Scientist, SLAC National Accelerator Laboratory

Bio

BIO

Dr. Abild-Pedersen is the acting 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)

Teaching

COURSES

2018-19

- Basic Principles of Heterogeneous Catalysis with Applications in Energy Transformations: CHEMENG 142, CHEMENG 242 (Spr)

Publications

PUBLICATIONS

- **Enhanced CO tolerance of Pt clusters supported on graphene with lattice vacancies** *PHYSICAL REVIEW B*
Hamamoto, Y., Wella, S., Inagaki, K., Abild-Pedersen, F., Bligaard, T., Hamada, I., Morikawa, Y.
2020; 102 (7)
- **Predicting metal-metal interactions. II. Accelerating generalized schemes through physical insights** *JOURNAL OF CHEMICAL PHYSICS*
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2020; 152 (9)

- **Predicting metal-metal interactions. I. The influence of strain on nanoparticle and metal adlayer stabilities** *JOURNAL OF CHEMICAL PHYSICS*
Streibel, V., Choksi, T. S., Abild-Pedersen, F.
2020; 152 (9)
- **Revealing the structure of a catalytic combustion active-site ensemble combining uniform nanocrystal catalysts and theory insights.** *Proceedings of the National Academy of Sciences of the United States of America*
Yang, A. C., Choksi, T., Streibel, V., Aljama, H., Wrasman, C. J., Roling, L. T., Goodman, E. D., Thomas, D., Bare, S. R., Sánchez-Carrera, R. S., Schäfer, A., Li, Y., Abild-Pedersen, et al
2020
- **Catalyst deactivation via decomposition into single atoms and the role of metal loading** *NATURE CATALYSIS*
Goodman, E. D., Johnston-Peck, A. C., Dietze, E. M., Wrasman, C. J., Hoffman, A. S., Abild-Pedersen, F., Bare, S. R., Plessow, P. N., Cargnello, M.
2019; 2 (9): 748–55
- **Single-atom species determine the deactivation of supported catalysts**
Cargnello, M., Goodman, E., Abild-Pedersen, F., Bare, S.
AMER CHEMICAL SOC.2019
- **Machine Learning for Computational Heterogeneous Catalysis** *CHEMCATCHEM*
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2019; 11 (16): 3579–99
- **Enhancing Electrocatalytic Water Splitting by Strain Engineering** *ADVANCED MATERIALS*
You, B., Tang, M. T., Tsai, C., Abild-Pedersen, F., Zheng, X., Li, H.
2019; 31 (17)
- **Predicting Adsorption Properties of Catalytic Descriptors on Bimetallic Nanoalloys with Site-Specific Precision** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
Choksi, T. S., Roling, L. T., Streibel, V., Abild-Pedersen, F.
2019; 10 (8): 1852–59
- **Revealing the Synergy between Oxide and Alloy Phases on the Performance of Bimetallic In-Pd Catalysts for CO₂ Hydrogenation to Methanol** *ACS CATALYSIS*
Snider, J. L., Streibel, V., Hubert, M. A., Choksi, T. S., Valle, E., Upham, D., Schumann, J., Duyar, M. S., Gallo, A., Abild-Pedersen, F., Jaramillo, T. F.
2019; 9 (4): 3399–3412
- **Density-dependent deactivation mechanism in supported catalysts by high-temperature decomposition of particles into single atoms**
Goodman, E., Johnston-Peck, A., Dietze, E., Wrasman, C., Hoffman, A., Abild-Pedersen, F., Bare, S., Plessow, P., Cargnello, M.
AMER CHEMICAL SOC.2019
- **Uncovering the details of methane combustion on palladium catalysts using well-defined nanocrystal precursors**
Cargnello, M., Huang, W., Goodman, E., Willis, J., Yang, A., Abild-Pedersen, F., Johnston-Peck, A., Bare, S.
AMER CHEMICAL SOC.2019
- **A coordination-based model for transition metal alloy nanoparticles** *NANOSCALE*
Roling, L. T., Choksi, T. S., Abild-Pedersen, F.
2019; 11 (10): 4438–52
- **Enhancing Electrocatalytic Water Splitting by Strain Engineering.** *Advanced materials (Deerfield Beach, Fla.)*
You, B., Tang, M. T., Tsai, C., Abild-Pedersen, F., Zheng, X., Li, H.
2019; e1807001
- **Accessing the C-C transition state energy on transition metals.** *Physical chemistry chemical physics : PCCP*
Aljama, H., Abild-Pedersen, F.
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- **Supported Catalyst Deactivation by Decomposition into Single Atoms Is Suppressed by Increasing Metal Loading.** *Nature catalysis*
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- **Understanding Structure-Property Relationships of MoO₃-Promoted Rh Catalysts for Syngas Conversion to Alcohols.** *Journal of the American Chemical Society*
Asundi, A. S., Hoffman, A. S., Bothra, P., Boubnov, A., Vila, F. D., Yang, N., Singh, J. A., Zeng, L., Raiford, J. A., Abild-Pedersen, F., Bare, S. R., Bent, S. F.
2019
- **Theoretical and Experimental Studies of CoGa Catalysts for the Hydrogenation of CO₂ to Methanol** *CATALYSIS LETTERS*
Singh, J. A., Cao, A., Schumann, J., Wang, T., Norskov, J. K., Abild-Pedersen, F., Bent, S. F.
2018; 148 (12): 3583–91
- **A Highly Active Molybdenum Phosphide Catalyst for Methanol Synthesis from CO and CO₂** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Duyar, M. S., Tsai, C., Snider, J. L., Singh, J. A., Gallo, A., Yoo, J., Medford, A. J., Abild-Pedersen, F., Studt, F., Kibsgaard, J., Bent, S. F., Norskov, J. K., Jaramillo, et al
2018; 57 (46): 15045–50
- **Mechanistic Insights into the Synthesis of Higher Alcohols from Syngas on CuCo Alloys** *ACS CATALYSIS*
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2018; 8 (11): 10148–55
- **Strongly Modified Scaling of CO Hydrogenation in Metal Supported TiO Nanostripes** *ACS CATALYSIS*
Sandberg, R. B., Hansen, M. H., Norskov, J. K., Abild-Pedersen, F., Bajdich, M.
2018; 8 (11): 10555–63
- **Tuning Methane Activation Chemistry on Alkaline Earth Metal Oxides by Doping** *JOURNAL OF PHYSICAL CHEMISTRY C*
Aljama, H., Norskov, J. K., Abild-Pedersen, F.
2018; 122 (39): 22544–48
- **Low-Temperature Methane Partial Oxidation to Syngas with Modular Nanocrystal Catalysts** *ACS APPLIED NANO MATERIALS*
Goodman, E. D., Latimer, A. A., Yang, A., Wu, L., Tahsini, N., Abild-Pedersen, F., Cargnello, M.
2018; 1 (9): 5258–67
- **Understanding and tuning catalytic materials using well-defined nanocrystal precursors**
Cargnello, M., Willis, J., Goodman, E., Wrasman, C., Yang, A., Abild-Pedersen, F., Bare, S.
AMER CHEMICAL SOC.2018
- **Well-defined nanocrystals catalysts as active phases and premier materials for spectroscopic studies of catalyst restructuring**
Cargnello, M., Goodman, E., Aitbekova, A., Wrasman, C., Riscoe, A., Yang, A., Abild-Pedersen, F., Bare, S.
AMER CHEMICAL SOC.2018
- **Theoretical Investigation of Methane Oxidation on Pd(111) and Other Metallic Surfaces** *JOURNAL OF PHYSICAL CHEMISTRY C*
Yoo, J., Schumann, J., Studt, F., Abild-Pedersen, F., Norskov, J. K.
2018; 122 (28): 16023–32
- **Nature of Lone-Pair-Surface Bonds and Their Scaling Relations** *INORGANIC CHEMISTRY*
Kakekhani, A., Roling, L. T., Kulkarni, A., Latimer, A. A., Abroshan, H., Schumann, J., Aljama, H., Siahrostami, S., Ismail-Beigi, S., Abild-Pedersen, F., Norskov, J. K.
2018; 57 (12): 7222–38
- **Structure-Sensitive Scaling Relations: Adsorption Energies from Surface Site Stability** *CHEMCATCHEM*
Roling, L. T., Abild-Pedersen, F.
2018; 10 (7): 1643–50
- **Selectivity of Synthesis Gas Conversion to C₂+ Oxygenates on fcc(111) Transition-Metal Surfaces** *ACS CATALYSIS*
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- **Selective catalysts for higher alcohol synthesis: A combined DFT and micro-kinetic modeling study**
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- **Mechanistic insights into the synthesis of higher alcohols from syngas on CuCo-alloys**

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- **Understanding and tuning catalytic materials For methane activation using nanocrystal precursors**
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- **Generic approach to access barriers in dehydrogenation reactions** *COMMUNICATIONS CHEMISTRY*
Yu, L., Vilella, L., Abild-Pedersen, F.
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- **Systematic Structure Property Relationship Studies in Palladium Catalyzed Methane Complete Combustion** *ACS CATALYSIS*
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2017; 7 (11): 7810–21
- **Configurational Energies of Nanoparticles Based on Metal-Metal Coordination** *JOURNAL OF PHYSICAL CHEMISTRY C*
Roling, L. T., Li, L., Abild-Pedersen, F.
2017; 121 (41): 23002–10
- **Investigating Catalyst-Support Interactions To Improve the Hydrogen Evolution Reaction Activity of Thiomolybdate [Mo₃S₁₃](2-) Nanoclusters** *ACS CATALYSIS*
Hellstern, T. R., Kibsgaard, J., Tsai, C., Palm, D. W., King, L. A., Abild-Pedersen, F., Jaramillo, T. F.
2017; 7 (10): 7126–30
- **Rh-MnO Interface Sites Formed by Atomic Layer Deposition Promote Syngas Conversion to Higher Oxygenates** *ACS CATALYSIS*
Yang, N., Yoo, J., Schumann, J., Bothra, P., Singh, J. A., Valle, E., Abild-Pedersen, F., Norskov, J. K., Bent, S. F.
2017; 7 (9): 5746–57
- **Theoretical Insights into Methane C-H Bond Activation on Alkaline Metal Oxides** *JOURNAL OF PHYSICAL CHEMISTRY C*
Aljama, H., Norskov, J. K., Abild-Pedersen, F.
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- **A Theoretical Study of Methanol Oxidation on RuO₂(110): Bridging the Pressure Gap** *ACS CATALYSIS*
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- **Electrochemical generation of sulfur vacancies in the basal plane of MoS₂ for hydrogen evolution** *NATURE COMMUNICATIONS*
Tsai, C., Li, H., Park, S., Park, J., Han, H. S., Norskov, J. K., Zheng, X., Abild-Pedersen, F.
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- **Theoretical study on oxidative coupling of methane using MgO**
Aljama, H., Norskov, J., Abild-Pedersen, F.
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- **Scaling Relations for Adsorption Energies on Doped Molybdenum Phosphide Surfaces** *ACS CATALYSIS*
Fields, M., Tsai, C., Chen, L. D., Abild-Pedersen, F., Norskov, J. K., Chan, K.
2017; 7 (4): 2528–2534
- **Modeling the Migration of Platinum Nanoparticles on Surfaces Using a Kinetic Monte Carlo Approach** *JOURNAL OF PHYSICAL CHEMISTRY C*
Li, L., Plessow, P. N., Rieger, M., Sauer, S., Sanchez-Carrera, R. S., Schaefer, A., Abild-Pedersen, F.
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- **Understanding trends in C-H bond activation in heterogeneous catalysis** *NATURE MATERIALS*
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- **Mechanistic insights into heterogeneous methane activation.** *Physical chemistry chemical physics*
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- **Bond Order Conservation Strategies in Catalysis Applied to the NH₃ Decomposition Reaction** *ACS CATALYSIS*
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- **Methanol Partial Oxidation on Ag(111) from First Principles** *CHEMCATCHEM*
Aljama, H., Yoo, J. S., Nørskov, J. K., Abild-Pedersen, F., Studt, F.
2016; 8 (23): 3621-3625
- **Direct and continuous strain control of catalysts with tunable battery electrode materials** *SCIENCE*
Wang, H., Xu, S., Tsai, C., Li, Y., Liu, C., Zhao, J., Liu, Y., Yuan, H., Abild-Pedersen, F., Prinz, F. B., Nørskov, J. K., Cui, Y.
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- **Understanding trends in C-H bond activation in heterogeneous catalysis.** *Nature materials*
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2016
- **Two-Dimensional Materials as Catalysts for Energy Conversion** *CATALYSIS LETTERS*
Siahrostami, S., Tsai, C., Karamad, M., Koitz, R., Garcia-Melchor, M., Bajdich, M., Vojvodic, A., Abild-Pedersen, F., Nørskov, J. K., Studt, F.
2016; 146 (10): 1917-1921
- **Sintering of Pt Nanoparticles via Volatile PtO₂: Simulation and Comparison with Experiments** *ACS CATALYSIS*
Plessow, P. N., Abild-Pedersen, F.
2016; 6 (10): 7098-7108
- **Elucidating the electronic structure of supported gold nanoparticles and its relevance to catalysis by means of hard X-ray photoelectron spectroscopy** *SURFACE SCIENCE*
Reinecke, B. N., Kuhl, K. P., Ogasawara, H., Li, L., Voss, J., Abild-Pedersen, F., Nilsson, A., Jaramillo, T. F.
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- **Dynamical Observation and Detailed Description of Catalysts under Strong Metal-Support Interaction** *NANO LETTERS*
Zhang, S., Plessow, P. N., Willis, J. J., Dai, S., Xu, M., Graham, G. W., Cargnello, M., Abild-Pedersen, F., Pan, X.
2016; 16 (7): 4528-4534
- **Modeling the Interface of Platinum and alpha-Quartz(001): Implications for Sintering** *JOURNAL OF PHYSICAL CHEMISTRY C*
Plessow, P. N., Sanchez-Carrera, R. S., Li, L., Rieger, M., Sauer, S., Schaefer, A., Abild-Pedersen, F.
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- **Trends in the Thermodynamic Stability of Ultrathin Supported Oxide Films** *JOURNAL OF PHYSICAL CHEMISTRY C*
Plessow, P. N., Bajdich, M., Greene, J., Vojvodic, A., Abild-Pedersen, F.
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- **Chemical and Phase Evolution of Amorphous Molybdenum Sulfide Catalysts for Electrochemical Hydrogen Production.** *ACS nano*
Lee, S. C., Benck, J. D., Tsai, C., Park, J., Koh, A. L., Abild-Pedersen, F., Jaramillo, T. F., Sinclair, R.
2016; 10 (1): 624-632
- **Activating and optimizing MoS₂ basal planes for hydrogen evolution through the formation of strained sulphur vacancies** *NATURE MATERIALS*
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Tsai, C., Chan, K., Nørskov, J. K., Abild-Pedersen, F.
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- **Surface Tension Effects on the Reactivity of Metal Nanoparticles** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
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- **Predicting Promoter-Induced Bond Activation on Solid Catalysts Using Elementary Bond Orders** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
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2015; 328: 36-42
- **Hydrogenation of CO₂ to methanol and CO on Cu/ZnO/Al₂O₃: Is there a common intermediate or not?** *JOURNAL OF CATALYSIS*
Kunkes, E. L., Studt, F., Abild-Pedersen, F., Schloegl, R., Behrens, M.
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- **Toward Controlled Growth of Helicity-Specific Carbon Nanotubes** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
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- **Examining the Linearity of Transition State Scaling Relations** *JOURNAL OF PHYSICAL CHEMISTRY C*
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- **The Mechanism of CO and CO₂ Hydrogenation to Methanol over Cu-Based Catalysts** *CHEMCATCHEM*
Studt, F., Behrens, M., Kunkes, E. L., Thomas, N., Zander, S., Tarasov, A., Schumann, J., Frei, E., Varley, J. B., Abild-Pedersen, F., Norskov, J. K., Schloegl, R.
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- **Catalyst design principles: An application to the steam reforming of methane**
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AMER CHEMICAL SOC.2015
- **Transition-metal doped edge sites in vertically aligned MoS₂ catalysts for enhanced hydrogen evolution** *NANO RESEARCH*
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- **On the role of the surface oxygen species during A-H (A = C, N, O) bond activation: a density functional theory study.** *Chemical communications*
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- **Energetics of the Water-Gas-Shift Reaction on the Active Sites of the Industrially Used Cu/ZnO/Al₂O₃ Catalyst** *CATALYSIS LETTERS*
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- **Insights into carbon nanotube nucleation: Cap formation governed by catalyst interfacial step flow** *SCIENTIFIC REPORTS*
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- **Discovery of a Ni-Ga catalyst for carbon dioxide reduction to methanol** *NATURE CHEMISTRY*
Studt, F., Sharafutdinov, I., Abild-Pedersen, F., Elkjaer, C. F., Hummelshøj, J. S., Dahl, S., Chorkendorff, I., Norskov, J. K.
2014; 6 (4): 320-324
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AMER CHEMICAL SOC.2014
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Medford, A. J., Lausche, A. C., Abild-Pedersen, F., Temel, B., Schjodt, N. C., Norskov, J. K., Studt, F.
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- **In silico search for novel methane steam reforming catalysts** *NEW JOURNAL OF PHYSICS*
Xu, Y., Lausche, A. C., Wang, S., Khan, T. S., Abild-Pedersen, F., Studt, F., Norskov, J. K., Bligaard, T.
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