Stanford

Kirsten T Winther

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Bio

BIO

The main goal of my research is to combine density functional theory simulations and data science approaches to accelerate the discovery of novel materials for catalysis. My research interests include:

- The development of machine learning models for the prediction of material stability and adsorption energetics
- Accelerated high-throughput frameworks for materials discovery, using machine-learning aided (active-learning) algorithms for materials exploration.
- Developing scientific software and the open database catalysis-hub.org.

Publications

PUBLICATIONS

- **Understanding the Electronic and Structural Effects in ORR Intermediate Binding on Anion-Substituted Zirconia Surfaces** *CHEMPHYSCHEM*
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- **Application of machine learning to discover new intermetallic catalysts for the hydrogen evolution and the oxygen reduction reactions** *CATALYSIS SCIENCE & TECHNOLOGY*
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  2024
- **Interpretable Machine Learning Models for Practical Antimonate Electrocatalyst Performance.** *Chemphyschem : a European journal of chemical physics and physical chemistry*
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- **Prediction of O and OH Adsorption on Transition Metal Oxide Surfaces from Bulk Descriptors** *ACS CATALYSIS*
  Comer, B. M., Bothra, N., Lunger, J. R., Abild-Pedersen, F., Bajdich, M., Winther, K. T.
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- **GPAW: An open Python package for electronic structure calculations** *JOURNAL OF CHEMICAL PHYSICS*
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- **Synergistic effects of mixing and strain in high entropy spinel oxides for oxygen evolution reaction.** *Nature communications*
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- **Efficient and Stable Acidic Water Oxidation Enabled by Low-Concentration, High-Valence Iridium Sites** *ACS ENERGY LETTERS*
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  2022
- **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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- **Theory-Aided Discovery of Metallic Catalysts for Selective Propane Dehydrogenation to Propylene** *ACS CATALYSIS*
  Wang, T., Cui, X., Winther, K. T., Abild-Pedersen, F., Bligaard, T., Norskov, J. K.
  2021; 11 (10): 6290-6297
- **A Bayesian framework for adsorption energy prediction on bimetallic alloy catalysts** *NPJ COMPUTATIONAL MATERIALS*
  Mamun, O., Winther, K. T., Boes, J. R., Bligaard, T.
  2020; 6 (1)
- **Active Learning Accelerated Discovery of Stable Iridium Oxide Polymorphs for the Oxygen Evolution Reaction** *CHEMISTRY OF MATERIALS*
  Flores, R. A., Paolucci, C., Winther, K. T., Jain, A., Torres, J., Aykol, M., Montoya, J., Norskov, J. K., Bajdich, M., Bligaard, T.
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- **Machine Learning for Computational Heterogeneous Catalysis** *CHEMCATCHEM*
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- **Catalysis-Hub.org, an open electronic structure database for surface reactions.** *Scientific data*
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  2019; 6 (1): 75
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- **Graph Theory Approach to High-Throughput Surface Adsorption Structure Generation** *JOURNAL OF PHYSICAL CHEMISTRY A*
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- **Graph Theory Approach to High-Throughput Surface Adsorption Structure Generation.** *The journal of physical chemistry. A*
  Boes, J. R., Mamun, O., Winther, K., Bligaard, T.
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