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Publications

PUBLICATIONS

- **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.
2020; 32 (13): 5854–63
- **Machine Learning for Computational Heterogeneous Catalysis** *CHEMCATCHEM*
Lamoureux, P., Winther, K. T., Torres, J., Streibel, V., Zhao, M., Bajdich, M., Abild-Pedersen, F., Bligaard, T.
2019; 11 (16): 3579–99
- **Catalysis-Hub.org, an open electronic structure database for surface reactions.** *Scientific data*
Winther, K. T., Hoffmann, M. J., Boes, J. R., Mamun, O., Bajdich, M., Bligaard, T.
2019; 6 (1): 75
- **High-throughput calculations of catalytic properties of bimetallic alloy surfaces.** *Scientific data*
Mamun, O., Winther, K. T., Boes, J. R., Bligaard, T.
2019; 6 (1): 76
- **Catalysis-hub.org: An open electronic structure database for surface reactions and catalytic materials**
Winther, K., Hoffmann, M., Mamun, O., Boes, J., Bajdich, M., Bligaard, T.
AMER CHEMICAL SOC.2019
- **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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