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LIST OF PUBLICATIONS

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2024

REVERSIBLE STRUCTURAL EVOLUTION OF METAL-NITROGEN-DOPED CARBON CATALYSTS DURING CO₂ ELECTROREDUCTION: AN OPERANDO X-RAY ABSORPTION SPECTROSCOPY STUDY.

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(highlighted in the virtual issue of The Journal of Physical Chemistry on Machine Learning)

DETERMINATION OF BIMETALLIC ARCHITECTURES IN NANOMETER-SCALE CATALYSTS BY COMBINING MOLECULAR DYNAMICS SIMULATIONS WITH X-RAY ABSORPTION SPECTROSCOPY

J. Timoshenko, K.R.Keller, A.I.Frenkel

J. Chem. Phys. 146, 114201 (2017)

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PROBING STRUCTURAL RELAXATION IN NANOSIZED CATALYSTS BY COMBINING EXAFS AND REVERSE MONTE CARLO METHODS

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