

• **List of publications: Dr. Nicolas Kaeffer**

2023

- Singh, A., Kemper, G., Weyhermuller, T., **Kaeffer, N.**, Leitner, W. (2023) Activated Mn-MACHO Complexes Form Stable CO₂ Adducts *Chemistry – A European Journal* <https://doi.org/10.1002/chem.202303438>
- Durin, G., **Kaeffer, N.**, Leitner, W. (2023) Electrocatalytic hydrogenation of unsaturated organic compounds with molecular complexes: Mechanistic views *Current Opinion in Electrochemistry* <https://doi.org/10.1016/j.coelec.2023.101371>
- Durin, G., Lee, M. Y., Pogany, M. A., Weyhermuller, T., **Kaeffer, N.**, Leitner, W. (2023) Hydride-Free Hydrogenation: Unraveling the Mechanism of Electrocatalytic Alkyne Semihydrogenation by Nickel-Bipyridine Complexes *Journal of the American Chemical Society* <https://doi.org/10.1021/jacs.3c03340>

2022

- Han, C. H., Zenner, J., Johny, J., **Kaeffer, N.**, Bordet, A., Leitner, W. (2022) Electrocatalytic hydrogenation of alkenes with Pd/carbon nanotubes at an oil-water interface *Nature Catalysis* <https://doi.org/10.1038/s41929-022-00882-4>
- Wang, Z., Volker, L. A., Robinson, T. C., **Kaeffer, N.**, Menzildjian, G., Jabbour, R., Venkatesh, A., Gajan, D., Rossini, A. J., Coperet, C., Lesage, A. (2022) Speciation and Structures in Pt Surface Sites Stabilized by N-Heterocyclic Carbene Ligands Revealed by Dynamic Nuclear Polarization Enhanced Indirectly Detected (195)Pt NMR Spectroscopic Signatures and Fingerprint Analysis *Journal of the American Chemical Society* <https://doi.org/10.1021/jacs.2c08300>
- **Kaeffer, N.**, Leitner, W. (2022) Electrocatalysis with Molecular Transition-Metal Complexes for Reductive Organic Synthesis *JACS Au* <https://doi.org/10.1021/jacsau.2c00031>
- Lee, M. Y., Kahl, C., **Kaeffer, N.**, Leitner, W. (2022) Electrocatalytic Semihydrogenation of Alkynes with [Ni(bpy)(3)](2) *JACS Au* <https://doi.org/10.1021/jacsau.1c00574>

2021

- Kinzel, N. W., Demirbas, D., Bill, E., Weyhermuller, T., Werle, C., **Kaeffer, N.**, Leitner, W. (2021) Systematic Variation of 3d Metal Centers in a Redox-Innocent Ligand Environment: Structures, Electrochemical Properties, and Carbon Dioxide Activation *Inorganic Chemistry* <https://doi.org/10.1021/acs.inorgchem.1c02909>

2020

- **Kaeffer, N.**, Mance, D., Coperet, C. (2020) N-Heterocyclic Carbene Coordination to Surface Copper Sites in Selective Semihydrogenation Catalysts from Solid-State NMR Spectroscopy *Angewandte Chemie International Edition* <https://doi.org/10.1002/anie.202006209>
- Lebedev, D., Ezhov, R., Heras-Domingo, J., Comas-Vives, A., **Kaeffer, N.**, Willinger, M., Solans-Monfort, X., Huang, X., Pushkar, Y., Coperet, C. (2020) Atomically Dispersed Iridium on Indium Tin Oxide Efficiently Catalyzes Water Oxidation *ACS Central Science* <https://doi.org/10.1021/acscentsci.0c00604>

2019

- Mavrokefalos, C. K., **Kaeffer, N.**, Liu, H. J., Krumeich, F., Copéret, C. (2019) Small and Narrowly Distributed Copper Nanoparticles Supported on Carbon Prepared by Surface Organometallic Chemistry for Selective Hydrogenation and CO₂ Electroconversion Processes *ChemCatChem* <https://doi.org/10.1002/cctc.201901414>

- Chandrasekaran, S., **Kaeffer, N.**, Cagnon, L., Aldakov, D., Fize, J., Nonglaton, G., Baleras, F., Mailley, P., Artero, V. (2019) A robust ALD-protected silicon-based hybrid photoelectrode for hydrogen evolution under aqueous conditions *Chemical Science* <https://doi.org/10.1039/c8sc05006f>

2018

- Kaeffer, N.**, Windle, C. D., Brisse, R., Gablin, C., Leonard, D., Jusselme, B., Chavarot-Kerlidou, M., Artero, V. (2018) Insights into the mechanism and aging of a noble-metal free H₂-evolving dye-sensitized photocathode *Chemical Science* <https://doi.org/10.1039/c8sc00899j>
- Kaeffer, N.**, Liu, H. J., Lo, H. K., Fedorov, A., Coperet, C. (2018) An N-heterocyclic carbene ligand promotes highly selective alkyne semihydrogenation with copper nanoparticles supported on passivated silica *Chemical Science* <https://doi.org/10.1039/c8sc01924j>
- Kaeffer, N.**, Larmier, K., Fedorov, A., Coperet, C. (2018) Origin of ligand-driven selectivity in alkyne semihydrogenation over silica-supported copper nanoparticles *Journal of Catalysis* <https://doi.org/10.1016/j.jcat.2018.06.006>
- Lebedev, D., Pineda-Galvan, Y., Tokimaru, Y., Fedorov, A., **Kaeffer, N.**, Coperet, C., Pushkar, Y. (2018) The Key Ru(V)=O Intermediate of Site-Isolated Mononuclear Water Oxidation Catalyst Detected by in Situ X-ray Absorption Spectroscopy *Journal of the American Chemical Society* <https://doi.org/10.1021/jacs.7b11388>

2016

- Coutard, N., **Kaeffer, N.**, Artero, V. (2016) Molecular engineered nanomaterials for catalytic hydrogen evolution and oxidation *Chemical Communications* <https://doi.org/10.1039/c6cc06311j>
- Sahara, G., Kumagai, H., Maeda, K., **Kaeffer, N.**, Artero, V., Higashi, M., Abe, R., Ishitani, O. (2016) Photoelectrochemical Reduction of CO₂ Coupled to Water Oxidation Using a Photocathode with a Ru(II)-Re(I) Complex Photocatalyst and a CoO(x)/TaON Photoanode *Journal of the American Chemical Society* <https://doi.org/10.1021/jacs.6b09212>
- Kaeffer, N.**, Massin, J., Lebrun, C., Renault, O., Chavarot-Kerlidou, M., Artero, V. (2016) Covalent Design for Dye-Sensitized H₂-Evolving Photocathodes Based on a Cobalt Diimine-Dioxime Catalyst *Journal of the American Chemical Society* <https://doi.org/10.1021/jacs.6b05865>
- Kaeffer, N.**, Morozan, A., Fize, J., Martinez, E., Guetaz, L., Artero, V. (2016) The Dark Side of Molecular Catalysis: Diimine–Dioxime Cobalt Complexes Are Not the Actual Hydrogen Evolution Electrocatalyst in Acidic Aqueous Solutions *ACS Catalysis* <https://doi.org/10.1021/acscatal.6b00378>
- Wood, C. J., Summers, G. H., Clark, C. A., **Kaeffer, N.**, Braeutigam, M., Carbone, L. R., D'Amario, L., Fan, K., Farre, Y., Narbey, S., Oswald, F., Stevens, L. A., Parmenter, C. D., Fay, M. W., La Torre, A., Snape, C. E., Dietzek, B., Dini, D., Hammarstrom, L., Pellegrin, Y., Odobel, F., Sun, L., Artero, V., Gibson, E. A. (2016) A comprehensive comparison of dye-sensitized NiO photocathodes for solar energy conversion *Physical Chemistry Chemical Physics* <https://doi.org/10.1039/c5cp05326a>

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- Kaeffer, N.**, Morozan, A., Artero, V. (2015) Oxygen Tolerance of a Molecular Engineered Cathode for Hydrogen Evolution Based on a Cobalt Diimine-Dioxime Catalyst *Journal of Physical Chemistry B* <https://doi.org/10.1021/acs.jpcc.5b03136>
- Queyriaux, N., **Kaeffer, N.**, Morozan, A., Chavarot-Kerlidou, M., Artero, V. (2015) Molecular cathode and photocathode materials for hydrogen evolution in photoelectrochemical devices

- Massin, J., Brautigam, M., **Kaeffer, N.**, Queyriaux, N., Field, M. J., Schacher, F. H., Popp, J., Chavarot-Kerlidou, M., Dietzek, B., Artero, V. (2015) Dye-sensitized PS-b-P2VP-templated nickel oxide films for photoelectrochemical applications *Interface Focus*
<https://doi.org/10.1098/rsfs.2014.0083>
- **Kaeffer, N.**, Chavarot-Kerlidou, M., Artero, V. (2015) Hydrogen evolution catalyzed by cobalt diimine-dioxime complexes *Accounts of Chemical Research*
<https://doi.org/10.1021/acs.accounts.5b00058>