Theoretical Insight into the Trends that Guide the Electrochemical Reduction of Carbon Dioxide to Formic Acid - DTU Orbit (26/03/2019)

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The electrochemical reduction (electroreduction) of CO$_2$ to formic acid (HCOOH) and its competing reactions, that is, the electroreduction of CO$_2$ to CO and the hydrogen evolution reaction (HER), on twenty-seven different metal surfaces have been investigated using density functional theory (DFT) calculations. Owing to a strong linear correlation between the free energies of COOH$^*$ and H$^*$, it seems highly unlikely that the electroreduction of CO$_2$ to HCOOH via the COOH$^*$ intermediate occurs without a large fraction of the current going to HER. On the other hand, the selective electroreduction of CO$_2$ to HCOOH seems plausible if the reaction occurs via the HCOO$^*$ intermediate, as there is little correlation between the free energies of HCOO$^*$ and H$^*$. Lead and silver surfaces are found to be the most promising monometallic catalysts showing high faradaic efficiencies for the electroreduction of CO$_2$ to HCOOH with small overpotentials. Our methodology is widely applicable, not only to metal surfaces, but also to other classes of materials enabling the computational search for electrocatalysts for CO$_2$ reduction to HCOOH.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic Scale Materials Modelling, SLAC National Accelerator Laboratory, Stanford University
Contributors: Yoo, J., Christensen, R., Vegge, T., Nørskov, J. K., Studt, F.
Pages: 358 – 363
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: ChemSusChem (Print)
Volume: 9
ISSN (Print): 1864-5631
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.86 SJR 2.538 SNIP 1.235
Web of Science (2017): Impact factor 7.411
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.505 SNIP 1.311
Web of Science (2016): Impact factor 7.226
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 7.33 SJR 2.53 SNIP 1.424
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 7.97 SJR 2.864 SNIP 1.663
Web of Science (2014): Impact factor 7.657
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 6.79 SJR 2.561 SNIP 1.46
Web of Science (2013): Impact factor 7.117
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 6.72 SJR 3.054 SNIP 1.553
Web of Science (2012): Impact factor 7.475
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): CiteScore 5.53 SJR 2.759 SNIP 1.497
Web of Science (2011): Impact factor 6.827