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2013-52/9 Kinetic Barriers 02 electroreduction

CO₂ electroreduction ...

... on copper is described by M. J. Janik, A. Asthagiri, and co-workers in their Communication on page 2459 ff. DFT calculations (incorporating the role of water solvation) of the activation barriers of elementary steps reveal a new path: Instead of proceeding through a CHO intermediate (which leads to methanol), methane formation goes through reduction of CO to COH, which eventually leads to CH_x species that can produce both methane and ethylene, as observed experimentally.



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