Theoretical calculation and spectroscopic measurements of electrocatalytic Cu and Cu/C thin films for CO2 reduction

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Research on selective CO_2 reduction catalysts that can be used in large-scale, low-cost and environmentally friendly ways is on the rise for some time. Especially with potential of capturing and reforming anthropogenic CO_2 into useful materials. Thus, a clear mechanism determination is necessary, which is still missing. Theoretical and experimental methods are used to find it, i.e. grain boundaries of Cu7 cluster investigated for electrocatalytic ability for the C_2H_4 formation through CH_2 dimerization or direct FTIR spectroscopy investigation for molecular-level information using an electrolysis cell with a thin film of copper cathode on the ATR crystal. It is known from theoretical calculations that electrochemical CO_2 reduction on Cu-decorated graphene electrode has attracted attention, because of its potential to generate significant amounts of hydrocarbon intermediates at high reaction rates over sustained periods of time. In fact, the first intermediate for ethylene is $-CO_2^-$, which can be further reduced via protonation to generate the -COOH intermediate that can be further reduced by one electron with one proton to form CO. But clear participation of graphene is not known.
In addition large-scale CO_2 reduction electrodes will be of composite structure not pure metal such as copper. Clear investigation of graphene material influence on the electrocatalytic CO_2 reduction process. Thus, semitransparent Cu and Cu/C thin films electrodes are deposited on the ATR crystal and spectroscopic investigation was done. The theoretical calculations are compared with spectroscopic data and conclusions on Cu and Cu/graphene role are made.

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