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**COMPUTATIONAL INVESTIGATION ON
ELECTROCHEMICAL REDUCTION OF CARBON DIOXIDE,
CARBOXYL AND FORMATE USING TIN AND LEAD
BIMETAL CATALYST**

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ABSTRACT

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Using density functional theory (DFT), this research focuses on how Sn, Pb, and Sn-Pb bimetallic catalysts can convert electrochemically reduce CO₂, COOH, and HCOO. This thesis provides a DFT-based computational analysis of the reaction mechanisms and catalytic properties of these materials on an atomic scale. Interaction energies, QTAIM, and charge population analyses were performed to evaluate the stability and character of the adsorption complexes. According to the results, HCOO has the strongest interaction with Sn and Pb surfaces, followed by COOH and CO₂, and Pb consistently has higher binding affinities for HCOO and COOH than Sn. Analysis of the bonding character between Pb-O and Sn-O revealed that most of the bonding is ionic with a moderate amount of covalency, which reflects a metal-oxygen coordination found in surface complexes. Charge redistribution data supports that HCOO is more stable when adsorbed onto Pb. These results demonstrate and support the synergistic interaction of Sn-Pb bimetallic materials for the selective and efficient transformation of CO₂ to HCOO, providing a theoretical framework for the development of high-performance electrocatalysts for the capture and utilization of carbon dioxide.

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