Computational Study of bimetallic dimers for Electrochemical CO$_2$ Reduction$^1$ CHRISTOPHER MORRISSEY, HAIYING HE, Valparaiso University, PETER ZAPOL, Argonne National Laboratory — CO$_2$ reduction requires a large energy input due to the high thermodynamic stability of CO$_2$. As a result, the challenge in CO$_2$ reduction is to find highly efficient, low costing catalysts. Recently, subnanometer metal clusters have shown promise as catalysts due to their unique electronic and catalytic properties. In this study, we have used density functional theory to study bimetallic dimers anchored on a defective graphene sheet for CO$_2$ reduction. Better performance were identified for some clusters. The results of this study will inform further experimental research in CO$_2$ reduction using subnanometer metal clusters.

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