# Search for $CO_2$ Reduction Reaction Catalysts: Computational Screening of Transition-Metal Dichalcogenides

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Due to the rapid development of modern society, the increasing energy demand and extreme climate change have been an uprising issue, and the electrochemical carbon dioxide reduction ($CO_2R$) can be a promising solution. Recently, $MoS_2$ was reported experimentally to produce 1-propanol as a major $CO_2R$ product, and it was also suggested computationally that S-vacancy is an active site on the basal plane. However, the intrinsic selectivity vs. HER was reported very low, and therefore, a search for catalysts with better properties is needed.

In this study, the anion vacancy on the basal plane of experimentally found 38 transition-metal dichalcogenides (TMDs) were computationally screened for $CO_2R$ catalytic performances. The focus is on catalysts that are predicted to produce HCHO, for it is the key intermediate for highly reduced species. Considering factors such as the theoretical onset potential, selectivity vs HER, and vacancy formation energy, $ReS_2$ and $ReSe_2$ were chosen to be promising candidates for HCHO production. This study can provide a higher understanding of $CO_2R$ catalysis and guidance to the discovery of novel materials.