Stress controlled CO_2 electrochemical reduction on copper

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We explore the ability of an applied stress, which leads to additional stress concentrations at step edges to synergistically modify active site properties responsible for the electrochemical conversion of CO_2 to hydrocarbons over Cu. This work requires the understanding of three interrelated effects: (i) the mechanical response of the defected surface to an applied stress, explored using embedded atom method (EAM) based molecular dynamics (MD) simulations to capture induced strains in realistic geometries; (ii) the chemical response of the defect site to localized distortion, probed using density functional theory (DFT) is used to compute the influence of stress on reaction intermediates; and (iii) the mapping of the stress to the chemical effect using the local step structures derived from the EAM-MD as input into an LCAO model and subsequently correlated to the DFT-determined electronic structure response. This study shows that stress may be used as a tool to control chemical intermediate binding energies and estimates the magnitude of the effect for electrochemical reduction of CO_2 on copper to form hydrocarbons.