**Selective CO2 conversion on low-dimensional materials**

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Conversion of carbon dioxide (CO2) to fuels and value-added chemicals is among the most promising approaches for reclaiming the major greenhouse gases to solve both energy and environmental issues. Developing catalysts composed of natural abundant, economical and eco-friendly elements is critical for industrialization of such technologies. Here we exploit a series of low-dimensional materials for CO2 conversion, including zero-dimensional (0D) metal-doped silicon cage clusters [1], two-dimensional (2D) silicene on Ag(111) substrate [2], and 2D ZnO ultrathin films [3]. By first-principles calculations, we show that the quantum size effect induces exotic surface states and catalytic behaviors for these silicon nanostructures and 2D oxide sheets. They exhibit remarkable activity for CO2 hydrogenation or reduction with water. The Si or O atoms serve as the reaction centers, with binding properties governed by the occupancy and energy level of p states of these non-metal atoms. The product selectivity depends on the size of Si clusters or the number of silicene or ZnO layers. Moreover, metal-doped Si clusters and 2D ZnO are able to harvest a large portion of sun light to drive the catalysis and reduce energy consumption. Our theoretical results provide vital guidelines for utilizing low-dimensional materials for selective CO2 conversion, and more importantly, we establish an explicit activity-band structure relationship for preciously tailoring the activity and selectivity of non-metal atoms.

**References**

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