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**Sequestration and selective oxidation of carbon monoxide on graphene edges** SUJATA PAUL, NC State University, ERIK E. SANTISO, MIT, MARCO B. NARDELLI, NC State University — The versatility of carbon nanostructures makes them attractive as possible catalytic materials, as they can be synthesized in various shapes and chemically modified by doping, functionalization, and the creation of defects in the nanostructure. In this work, we consider the carbon-mediated partial sequestration and selective oxidation of carbon monoxide (CO), an important problem in environmental chemistry and energy conversion. Using first principle calculations we study the key reactions of CO with carbon nanostructures, where the active sites can be regenerated by the deposition of carbon decomposed from the reactant (CO) to make the reactions self sustained. Carbon-mediated CO sequestration produces half of the CO<sub>2</sub> compared to the direct oxidation of CO, which is used in the cleaning of automobile gas. Furthermore, the carbon-mediated oxidation of CO to CO<sub>2</sub> is selectively favored when hydrogen is present, and could be used to purify hydrogen for use in fuel cells.

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