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Manipulation of Single Oxygen Vacancies on TiO_2(110) DANDA ACHARYA, PETER SUTTER, Brookhaven National Laboratory — Oxygen vacancies are among the primary chemically active defects on the surface of reducible transition metal oxides, playing a key role in surface chemistry, catalysis, and photocatalysis. We report the controlled manipulation of individual O-vacancies on reduced TiO_2(110)-1x1 using a low temperature scanning tunneling microscope. Localized voltage pulses trigger the hopping of single vacancies along a bridging oxygen (O_{br}) row. We discuss the microscopic manipulation mechanism and demonstrate atomic-scale control by constructing linear and more complex arrangements of vacancies. Single defect manipulation is used to probe the interaction of closely spaced vacancies, and to establish the possibility of forming highly reactive double and a triple O-vacancy clusters. Detailed experimental and theoretical analysis reveals that bridge-bonded O-vacancy pairs are stable and have lower energy than pairs of vacancies separated by two or more lattice spacings. The existence of stable vacancy pairs with exposed low-coordinated Ti atoms has implications on the reactivity of TiO_2(110) and of similar metal oxide surfaces.

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