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Effect of N- and P-Type Doping on the Oxygen-Binding Energy and Oxygen Spillover of Supported Palladium Clusters[1] ARTHUR C. REBER, SHIV N. KHANNA, Virginia Commonwealth University — The oxygen-binding energy is one of the primary factors determining catalytic activity in oxidation reactions. One strategy for controlling the binding of a reactant to a surface is to dope the surface to create complementary donor–acceptor pairs. As oxygen is an acceptor, we have investigated the effect of doping on the oxygen-binding energy on Pd atoms and clusters supported on a rutile TiO_2(110) surface. We find that the P-type doping of the TiO_2 surface dramatically reduces the O-binding energy to Pd. When extended to Pd_4-supported clusters, we find that the P-type dopant decreases the energy for the oxygen to bind at spillover sites directly to the TiO_2 surface. In Pd_4O_2, the oxygen-binding energy is reduced with P-type doping, suggesting that this strategy may be used to control the oxygen-binding energy to supported catalysts.

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