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A Coupling Mechanism between Co-doped Acceptors and its Control on Optical Absorption Edge of TiO2[1] WEI LI, SHIHAO WEI, XIANGMEI DUAN, Ningbo Univertsity — A hole-strain-mediated coupling between dopants in anatase TiO_2 is revealed by first-principles calculations. When the dopant complex on neighboring oxygen sites contains a large radius atom, and the doped system has at least one net hole, the dopants will strongly couple to form a pair through the local lattice strain induced by the large dopant. The coupling results in bandgap narrowing due to the appearance of the fully occupied mid-gap states, leading to a much more effective band gap reduction than that induced by mono-doping or conventional donor-acceptor codoping. The calculated absorption spectra show that acceptor-acceptor codopings could shift the absorption edge to the visible light region.

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