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Quantum Confinement and Surface Relaxation Effects in Rutile TiO_2 Nanowires[1] ABRAHAM HMIEL, YONGQIANG XUE, College of Nanoscale Science and Engineering, State University of New York at Albany — Recent developments in synthesis of TiO_2 nanowires with diameters on the atomic scale have opened up new grounds for studying structure-property relationships in the regime where quantum confinement effects are important. In the sub-nanometer range, the properties of nanowires can be sensitive to atomic-level control of surface morphology, functionalization, and nanowire stoichiometry during the growth and fabrication processes, thereby opening the way for new applications. First-principles density functional theory calculations have been applied to investigate the size- and shape-dependent properties of [001]-oriented rutile TiO_2 nanowires of rectangular cross section. We find that the pronounced oscillation in the formation energy and band structure of the nanowires as a function of the number of TiO_2 trilayers is largely connected to the presence or absence of a mirror Ti-O plane along each confinement direction. We demonstrate that the relative stability and the indirect or direct character of the band structure of the rutile TiO_2 nanowires arise from the interplay between surface relaxation and quantum confinement effects that depend on the even-odd parity of the number of TiO_2 trilayers.

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