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Effective strain-induced band gap narrowing of anatase TiO2: A soft crystal direction WAN-JIAN YIN, XIN-GAO GONG, Department of Physics, Fudan University, Shanghai, SU-HUAI WEI, National Renewable Energy Lab — TiO2 is one of the promising materials for photoelectrochemical hydrogen production through water splitting. However, due to its large band gap (3.2. eV), it cannot absorb sun light effectively. To reduce its band gap, various approaches have been attempted, including applying strain. Using first-principles band structure method, we have studied the electronic and elastic properties of TiO2 with anatase and rutile phases. We calculated the band gap deformation potentials of both phases under hydrostatic, epitaxial and uniaxial strains. We find that the hydrostatic deformation potential of TiO2 is small. However, unlike the rutile phase, there is a soft direction in anatase phase. By applying strain in this soft direction, we show that the band gap of anatase TiO2 could be narrowed effectively, thus, offering an opportunity to reduce the band gap of TiO2. We demonstrate that this approach of tuning the band gap by applying strain along soft direction of a layered semiconductor is general and should be applicable to other anisotropic energy-related materials.

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