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Engineering Oxygen Vacancy Distribution by Exteranl Strain DA-JUN SHU, SHU-TING GE, MU WANG, NAI-BEN MING, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China — The most common defects on surfaces of transition metal oxides are oxygen vacancies, which play critical roles in applications such as heterogeneous catalysis, photoelectrolysis, biocompatibility, etc.. If the nature and distribution of the oxygen vacancies can be controlled, the surface properties will then be modified for different applications. For this purpose, one needs to understand both the influence of oxygen vacancies on the surface properties and the responses of oxygen vacancies to different external fields. We have conducted comprehensive first principles calculations on the surface energy of strained rutile TiO2(110) with oxygen vacancies. The formation energy of each type of oxygen vacancy is calculated as a function of external strain. We find that the type of the most easily formed oxygen vacancy can be tuned by the strain and therefore suggest that the distribution of oxygen vacancies can be engineered by external strain, which helps to improve the applications of TiO2 surface where oxygen vacancies play important roles. The dependence of surface elastic properties on the type of oxygen vacancy is found to be responsible for the interplay between external strain and oxygen vacancies.

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