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Strain effect on diffusion properties of oxygen vacancies in bulk and subsurface of rutile TiO2[1] DAJUN SHU, ZHAOWU WANG, MU WANG, Shool of Physics, Nanjing University — The influences of external strain on diffusion properties of the bulk and subsurface oxygen vacancy (OV) in rutile TiO_2 are systematically studied using first-principle calculations. For OVs in bulk, we find that tensile (compressive) strain applied in the [001] direction or isotropically applied in the equivalent [110] and [$1\bar{1}0$] directions reduces (increases) the energy barriers of diffusion. Anisotropic strain applied in [110] and [$1\bar{1}0$] increases the energy barriers of diffusion in the two directions. Meanwhile it results in anisotropic diffusion behaviors. Between [110] and [$1\bar{1}0$], the bulk OV prefers to diffuse along the one in which more compressive or less tensile strain is applied. From subsurface to surface, the most energetically favorable OV pathway is along the [110] rows terminated with the surface bridging oxygen atoms. The diffusion barrier of the OV in the first trilayer is much lower than that of a bulk OV. External in-plane tensile strain can further reduce the energy barrier of the subsurface OV diffusion, and thus help to improve the diffusion of OVs from bulk to surface.

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