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Dopant induced surface reconstruction in N-doped rutile TiO_2(110) MATTHIAS BATZILL, Tulane University, ERIE MORALES, ULRIKE DIEBOLD — Recently N-doping of TiO_2 has attracted some attention because it has been demonstrated to shift the photocatalytic activity of TiO_2 from the UV-region to the visible light. Here we examine the impact of N-doping on the electronic structure and surface morphology of single crystal TiO_2 surfaces.* Often it is assumed that bulk dopants have little influence on the surface properties. In the case of rutile TiO_2(110) it is, however, well established that intrinsic O-vacancies cause the surface to reconstruct to form a 1x2 superstructure. We find that N-doping reduces the formation energy of O-vacancies in TiO_2 and as a consequence destabilizes the surface to cause a 1x2 reconstruction. Similar surface effects may be expected for other bulk dopants that are know to induce oxygen vacancies in TiO_2. * M. Batzill, E.H. Morales, U. Diebold, Phys. Rev. Lett. accepted

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