All-electron *GW* calculation of the electronic structure in light-element-doped TiO_2

Ryoji Sahara,[1*] Takashi Ishikawa,[2] Kaoru Ohno,[1,3]
Kyosuke Ueda,[2] and Takayuki Narushima [2]

[1] Research Center for Structural Materials, National Institute for Materials Science, Tsukuba, Japan; [2] Department of Materials Processing, Tohoku University, Sendai, Japan; [3] Graduate School of Engineering, Yokohama National University, Yokohama, Japan;
SAHARA.Ryoji@nims.go.jp

TiO_2 is known as a photocatalytic material, and its band gap corresponds to the UV region[1]. Adding visible-light responsive photocatalytic functionality to TiO_2 by doping impurity elements such as C and N can promote its technological applicability. An example is the TiO_2 coating on Ti dental implants to achieve antibacterial properties, which are induced by its photocatalytic reactions[2].

With the aim of investigating anatase and rutile TiO_2 doped with C, N, phase stability was first analyzed using density functional theory calculations considering interstitial and substitutional positions and oxygen vacancy(ies) at 700K (anatase) and at 1,000K (rutile). The stable defect states were found to depend on the oxygen (O_2) pressure conditions or oxygen chemical potential for C and N monodoped and codoped TiO_2 systems.

Thereafter, using TOMBO (TOhoku Mixed Basis Orbitals ab initio program)[3], the all-electron *GW* approach based on the manybody perturbation theory was adopted to determine the electronic structures of the stable systems and understand the mechanism of band gap narrowing, which originates from impurity doping under widely different oxygen pressure conditions. It is found that the band gap can be controlled by the oxygen chemical potential and doping states. Among various models, C and N codoped anatase TiO_2 under intermediate oxygen pressure shows a band gap of 2.28 eV, while, N doped rutile TiO_2 under high pressure shows a band gap of 1.86 eV. These materials can be used as photocatalyst for visible light [4,5].

References

1. Fujishima, A.; Honda, K. *Nature* **1972**, 238, 37-38.
2. Ueda, T.; Sato, N.; Koizumi, R.; Ueda, K.; Ito, K.; Ogasawara, K.; Narushima, T. *Dent. Mater.* **2021**, 37, e37-e46.
3. Ono, S.; Noguchi, Y.; Sahara, R.; Kawazoe, Y.; Ohno, K. *Comput. Phys. Commun.* **2015**, 189, 20-30.
4. Ishikawa, T.; Sahara, R.; Ohno, K.; Ueda, K.; Narushima, T. *Comput. Mater. Sci.* **2023**, 220, 112059.
5. Ishikawa, T.; Sahara, R.; Ohno, K.; Ueda, K.; Narushima, T. in submission.