

All-electron *GW* calculation of the electronic structure in light-element-doped TiO₂

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TiO₂ is known as a photocatalytic material, and its band gap corresponds to the UV region¹. Adding visible-light responsive photocatalytic functionality to TiO₂ by doping impurity elements such as C and N can promote its technological applicability. An example is the TiO₂ coating on Ti dental implants to achieve antibacterial properties, which are induced by its photocatalytic reactions².

With the aim of investigating anatase and rutile TiO₂ 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 (O₂) pressure conditions or oxygen chemical potential for C and N monodoped and codoped TiO₂ 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 TiO₂ under intermediate oxygen pressure shows a band gap of 2.28 eV, while, N doped rutile TiO₂ under high pressure shows a band gap of 1.86 eV. These materials can be used as photocatalyst for visible light^{4,5}.

References

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