**Energetics and optical properties of carbon impurities**

**in rutile TiO2**

Supparat Charoenphon,1 Adisak Boonchun1,2, and Pakpoom Reunchan,1,2\*

*1Department of Physics, Faculty of Science, Kasetsart University,*

*Bangkok 10900, Thailand*

*2Thailand Center of Excellence in physics (ThEP Center), Commission on Higher Education, Bangkok 10400, Thailand*

\* E-mail: pakpoom.r@ku.ac.th

Titanium dioxide (TiO2) is one of the most promising materials for many applications such as solar-cell system and photocatalysis. Non-metal doping of TiO2 is widely used to improve the photoconversion of the material by shifting the absorption edge from UV to visible-light region [1, 2]. Here, we employ hybrid density-functional calculations to investigate the energetics and electronic structures of carbon (C) impurities in rutile TiO2. The predominant configurations of C impurities under the O-poor and O-rich growth conditions are identified through the calculated formation energies. Under the O-poor condition, we find the substitutional C occupying oxygen site (CO), as shown in FIG. 1, is energetically favorable for Fermi-level values near the conduction band minimum (*n*-type TiO2) where it acts as double acceptor. On the other hand, when Fermi-level positions decrease toward the valence band, C atoms favor to form the C*i*-*V*O complex, as shown in FIG. 2, acting as sextuple donor. Under the O-rich condition, the C*i*-*V*Ti complex is found to be energetically favorable in *n*-type TiO2, and is exclusively stable in charge neutral. Our calculations based on the configuration coordinated diagram suggest that CO is an origin of visible light absorbtion in *n*-type rutile TiO2 fabricated under oxygen deflicient growth condition.

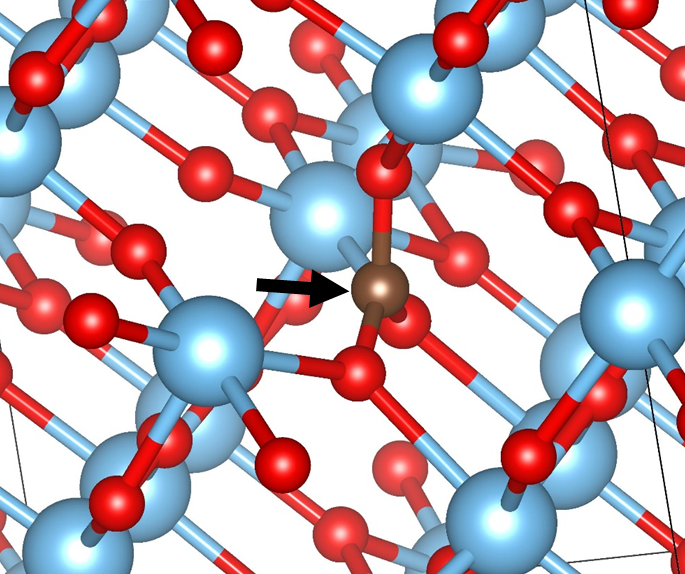
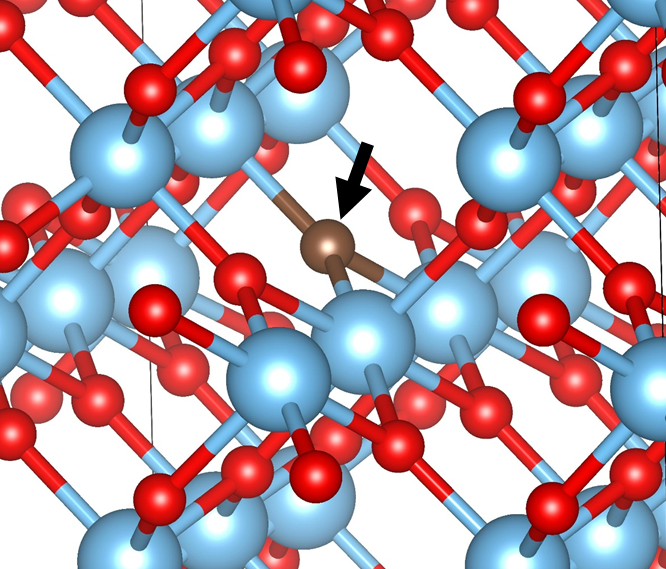


FIG. 2. (Color online) Local atomic configuration of the C*i*-*V*Ti complex. The interstitial C is indicated by the arrow.

FIG. 1. (Color online) Local atomic configuration of the substitutional C occupying O site (CO) in rutile TiO2. The substitutional C is indicated by the arrow [Ti: blue, O: red, C: dark brown].

[1]  Asahi, R.; Morikawa, T.; Ohwaki, T.; Aoki, K.; Taga, Y. *Science* **2001**, *293*, 269.

[2]  Khan, S. U. M.; Al-Shahry, M.; Ingler, W. B., Jr. *Science* **2002**, *297*, 2243.