ACCMS-Global Research Center
SRMIST, Chennai India

Webinar #24

Dr. Ryoji Sahara

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Title: All-electron GW approach for light-element-doped anatase TiO_2 using TOMBO

Registration link: http://tinyurl.com/33tzvvxh
**Zoom details will be shared with the registered participants*

Short biography

Dr. Ryoji Sahara is a Principal Researcher at Research Center for Structural Materials, National Institute for Materials Science (NIMS) in Japan since 2013. He is a group leader of Computational Structural Materials Group in the Center. He specializes in computational materials science through first-principles calculations.

Currently, his main interest is in designing structural materials with high strength at high temperature regions and providing a variety of functionalities by first-principles calculations, including to clarify chemical reactions at the surface and inside of materials, and designing microstructures of materials based on multiscale simulations such as first-principles phase field modelling.

Dr. Ryoji Sahara completed his doctoral studies in the Department of Materials Science at Tohoku University in Japan in March 2000. After that, he held various positions at School of Engineering and Institute for Materials Research, including Assistant Professor and Associate Professor.

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Abstract

TiO_2 is renowned as a photocatalytic material with a band gap situated in the UV region. Enhancing its applicability by imparting visible-light responsiveness through doping with impurity elements like C and N could significantly advance its technological utility. An application is the coating of Ti dental implants with TiO2 to attain antibacterial properties, induced by its photocatalytic reactions.

To explore the anatase TiO_2 doped with C and N, we first conducted an analysis of phase stability using density functional theory calculations. This analysis considered various defects in various positions including interstitial and substitutional, and accounted for oxygen vacancy(ies). The stable defect states were found to be contingent on the oxygen (O_2) pressure conditions or oxygen chemical potential for both C and N monodoped and codoped TiO_2 systems.

Subsequently, we employed TOMBO (TOhoku Mixed Basis Orbitals ab initio program) to perform the all-electron GW calculations based on many-body perturbation theory. This allowed us to determine the electronic structures of the stable systems and comprehend the mechanism behind the band gap narrowing resulting from impurity doping under varying oxygen pressure conditions. It is evident that the band gap can be manipulated by adjusting the oxygen chemical potential and doping states. Notably, C and N codoping proves more effective in narrowing the band gap compared to mono doping with either C or N.

Among the diverse systems studied, C and N codoped TiO_2 under intermediate oxygen pressure conditions exhibited the smallest band gap, measuring 2.28 eV. Consequently, it can be considered a promising material for visible light response photocatalysis.

Panelist

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