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触媒化学融合研究センター特別講演会

産総研触媒化学融合研究センターでは、様々な分野で活躍している大学、公的研究機関、企業等の方々をお招きして講演会を開催することで分野の垣根を越えた連携の実現を目指しています。多くの方々のご参加をお待ちしております。

“Strongly Facet-Dependent Properties of Semiconductor Crystals”

＜講師＞

National Tsing Hua University
Michael H. Huang

日時：2019年1月24日（木）15：30～17：00
場所：産総研第5事業所 第2本館
第4会議室（5-2　6603室）

＜講演概要＞

Our extensive investigations on the various properties of Cu_2O, Ag_2O, PbS, and Ag_3PO_4 crystals have shown they possess facet-dependent photocatalytic activity, electrical conductivity, and optical properties.[1] For example, {110}-bound Cu_2O rhombic dodecahedra are more photocatalytically active than {111}-bound Cu_2O octahedra, but {100}-bound cubes are inactive. Deposition of ZnO, CdS, and other semiconductor nanostructures on these Cu_2O polyhedra can often lead to partial or complete photocatalytic activity suppression despite their favorable bulk band energy alignment. This happens because facet effects should be extended to semiconductor interfaces, and frequently interfacial band bending can make photoexcited charge transfer across the interfaces becomes unfavorable. For electrical conductivity properties, a Cu_2O octahedron is highly conductive like a metal, a cube behaves like a semiconductor, while a rhombic dodecahedron is an insulator. The existence of a thin surface layer with dissimilar band structures for different crystal surfaces and thus different degrees of band bending at the crystal surfaces can explain these facet-dependent observations. Recently, we have shown Si and Ge wafers also possess facet-dependent electrical conductivity behaviors.[2,3] We have also synthesized size-tunable Cu_2O cubes, octahedra, and rhombic dodecahedra to demonstrate their possession of size- and facet-dependent light absorption and emission properties.[4] This means band diagram of semiconductors must be modified to account for size and facet effects. All these properties are related. Bond length, bond geometry, and frontier orbital electron distributions within in the ultrathin Si and Ge surface layers are different from those of the bulk, showing semiconductor facet effects should have quantum mechanical basis at the orbital level.

References

[1] Huang, M. H.; Naresh, G.; Chen, H.-S. Facet-Dependent Electrical, Photocatalytic, and Optical Properties of Semiconductor Crystals and Their Implications for Applications. *ACS Appl. Mater. Interfaces* **2018**, *10*, 4-15. [2] Tan, C.-S.; Huang, M. H. Silicon Wafers with Facet-Dependent Electrical Conductivity Properties. *Angew. Chem. Int. Ed.* **2017**, *56*, 15339-15343. [3] Hsieh, P.-L.; Lee, A.-T.; Chen, L.-J.; Huang, M. H. Germanium Wafers Possessing Facet-Dependent Electrical Conductivity Properties. *Angew. Chem. Int. Ed.* **2018**, *57*, 16162. [3] Huang, J.-Y.; Madasu, M.; Huang, M. H. Modified Semiconductor Band Diagrams Constructed from Optical Characterization of Size-Tunable Cu_2O Cubes, Octahedra, and Rhombic Dodecahedra. *J. Phys. Chem. C* **2018**, *122*, 13027-13033.

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