Contribution ID: **93** Type: **Oral Presentation**

FIRST PRINCIPLE STUDY OF HEMATITE (α-Fe2O3) SURFACES STRUCTURE DOPED WITH TRANSITION METALS

Tuesday, 9 July 2019 10:40 (20 minutes)

The photocatalytic water oxidation activity of hematite (α-Fe2O3) has been greatly enhanced by incorporating hematite nanoparticles on the reduced graphene oxide (rGO) nanosheets. Photoelectrochemical measurement results show that coupling the hematite nanoparticles with the rGO greatly increases the photocurrent and reduces the charge recombination rate. Transient absorption spectroscopy and time-domain terahertz spectroscopy have provided the direct evidence that the photogenerated electrons have transferred as the mobile carriers from α-Fe2O3 to rGO, which enhances the charge separation and suppresses the charge recombination. The conduction band edge of α -Fe2O3 is highly localized, leading to a heavy electron effective mass and, therefore, very low electron conductivity. Density functional theory was employed to study electronic and optical properties of doped hematite with transition metals. The results showed that the incorporation of Ti and Cr reduces the electron effective mass, which improve the electron conductivity of α-Fe2O3.

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yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

MSc

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Session Classification: Applied Physics

Track Classification: Track F - Applied Physics