Band-gap measurements of bulk and nanoscale hematite by soft x-ray spectroscopy - DTU Orbit (11/01/2019)

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Chemical and photochemical processes at semiconductor surfaces are highly influenced by the size of the band gap, and ability to control the band gap by particle size in nanomaterials is part of their promise. The combination of soft x-ray absorption and emission spectroscopies provides band-gap determination in bulk and nanoscale itinerant electron semiconductors such as CdS and ZnO, but this approach has not been established for materials such as iron oxides that possess band-edge electronic structure dominated by electron correlations. We performed soft x-ray spectroscopy at the oxygen K-edge to reveal band-edge electronic structure of bulk and nanoscale hematite. Good agreement is found between the hematite band gap derived from optical spectroscopy and the energy separation of the first inflection points in the x-ray absorption and emission onset regions. By applying this method to two sizes of phase-pure hematite nanoparticles, we find that there is no evidence for size-driven change in the band gap of hematite nanoparticles down to around 8 nm.

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