DIRECT OBSERVATION OF EXCITON DISSOCIATION AND CHARGE INJECTION: THE FIRST-STEP IN SOLAR ENERGY CONVERSION TECHNOLOGIES

SOMNATH BISWAS, JAKUB HUSEK, STEPHEN LONDO, ELIZABETH A FUGATE, ROBERT BAKER, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH, USA.*

Understanding the mechanism of interfacial hole transfer and the chemical nature of the hole acceptor state in NiO based solar materials are important for the rational design of devices with improved efficiency. NiO is widely utilized as a hole transport layer in solar energy devices. However, due to its complex electronic structure, the chemical nature of the hole acceptor state has remained an open question, despite the fact that hole localization in NiO significantly influences device efficiency. To comment on this, we present results of ultrafast charge carrier dynamics in a NiO based model heterojunction (Fe_2O_3/NiO) using extreme ultraviolet reflection-absorption (XUV-RA) spectroscopy. Element specific XUV-RA demonstrates the formation of transient Ni^{3+} within a few ps following selective photoexcition of the underlying Fe_2O_3 substrate. This indicates that fast hole transfer in this system occurs to NiO valence band states composed of significant Ni $3d$ character. Additionally, we show that this hole injection process proceeds via a two-step sequential mechanism where fast field driven exciton dissociation occurs in Fe_2O_3 in 680 ± 60 fs, followed by subsequent hole injection to NiO in 9.2 ± 2.9 ps. These results reveal the chemical nature of the hole acceptor state in widely used NiO hole transport layers and provides a direct observation of exciton dissociation and interfacial hole transfer in this system.