OBSERVATION OF ELECTRONIC AND STRUCTURAL INTERACTION BETWEEN SMALL POLARONS AND HOST MATERIALS USING FEMTOSECOND XUV REFLECTION SPECTROSCOPY

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Small polaron formation in transition metal oxides is believed to be a reaction bottleneck in many solar energy conversion applications. While polaron formation has been previously confirmed, the microscopic interaction between a small polaron and its host material is largely unexplored. Here, using femtosecond XUV reflection spectroscopy, we report the evidence of electronic and structural interaction between the small polaron and its host material in $CuFeO_2$, a photoelectrode material for CO_2 reduction. Initial small polaron formation is observed as a spectral blue shift occurring within the first 100 fs. After polaron formation, we observe an increased coherent oscillation signal around the polaron sites, which is attributed to polaron-induced optical phonons. This observation suggests that the polaron-associated local lattice distortion can launch optical phonons in neighboring unit cells. In addition to structural coupling, the electronic states in the host materials can also be modified during polaron formation. As an example, we report an increase of Fe oxidation states after photoexcitation. The population of these highly oxidized Fe atoms strongly correlates with polaron dynamics, suggesting that a polaron can alter its surrounding electronic states in host materials.