

Abstract Submitted
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Organic radical formation over transition metal oxides: Bonding trends studied with inelastic neutron scattering MATTHEW PATTERSON, Department of Chemistry, Louisiana State University, RICHARD KURTZ, Department of Physics and Astronomy, Louisiana State University, RANDALL HALL, Department of Natural Sciences and Mathematics, Dominican University of California, ERWIN POLIAKOFF, Department of Chemistry, Louisiana State University, PHILLIP SPRUNGER, Department of Physics and Astronomy, Louisiana State University — Environmentally persistent free radicals (EPFRs), a class of long-lived pollutants (lifetimes of 1-1000 hours) consisting of aromatic molecules chemisorbed to metal oxide-containing particulate matter, have significant public health impacts, having been demonstrated to produce pulmonary and cardiovascular dysfunction in animal models. Oxides of many environmentally abundant first-row transition metals form EPFRs, so a fundamental understanding of their formation mechanisms is crucial in developing strategies for their prevention and remediation. On most metal oxides, EPFRs form through electron transfer from an adsorbed organic such as phenol to a metal cation, reducing the cation; however, we demonstrate here that the opposite process uniquely occurs in ZnO, in which electrons are transferred from Zn to the adsorbed phenoxy group, creating the longest-lived known EPFR species. Using inelastic neutron scattering, we have probed vibrational excitations in model EPFR systems – chemisorbed phenol on ZnO, CuO, Fe₂O₃, and TiO₂ nanoparticles – in order to correlate their vibronic structure with known trends in their electronic structure and lifetimes.

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