NSF Highlights

Copper Oxide-Clusters Model of Persistent Free Radical Formation: A computational Approach

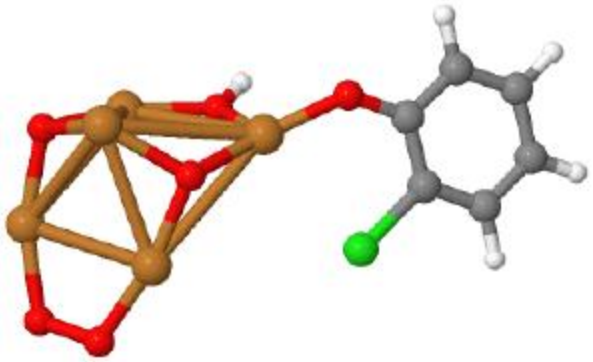

Figure 1: Copper oxide nanoparticle with bound dioxin/furan precursor. Credit: Randall Hall, Louisiana State University

Outcome/ Accomplishments

Environmentally hazardous compounds, such as polychlorinated dibenzo-p-dioxins and dibenzofurans, are formed during combustion from a variety of sources. The role of metal oxide-containing nanoparticles in pollutant formation is being characterized using computational studies of small metal oxide particles and a variety of experimental methods.

Impact/ Benefits

Hazardous waste incinerators, auto exhaust, and cigarette smoke are among the combustion sources that can form dioxins and furans on particles small enough to be inhaled by humans. This study aims to identify the mechanism of their formation with the goal of developing procedures to prevent or hinder the formation reactions.

Background

The adsorption of dioxin and furan precursors to the surface of metal oxide nanoparticles has been implicated as a crucial first step in the formation of dioxins and furans. Environmentally persistent free radicals are formed on these small particles, which can be inhaled deep into human lungs and cause cardiopulmonary disease. These initial steps can be quantified experimentally (Figure 2) and modeled with computational methods (Figure 1). Computational studies, when combined with experimental verification, offer the possibility of identifying the reaction site on the nanoparticles. Both dioxin and free radical formation can be better understood so that their formation and human exposure can be minimized.

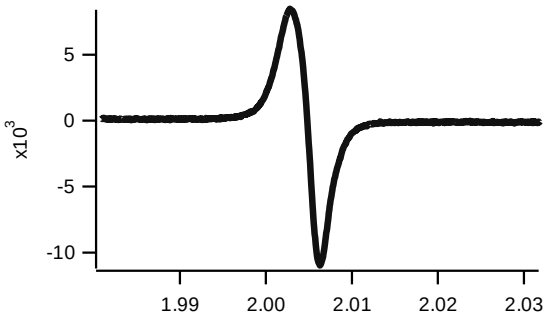

Figure 2. Electron paramagnetic spectrum of 2-chlorophenol adsorbed in 5%CuO/SiO_2 showing the presence of a furan/dioxin precursor bound to the surface of a metal oxide. Credit: Barry Dellinger, Louisiana State University.