

How to tame your beamline: Unwanted effects of X-rays in surface grafted copper (II) organometallics and copper exchanged zeolites, how they manifest, and what can be done about them?

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Abstract

Copper (II) containing materials are widely studied for a very diverse array of applications from biology, thorough catalysis, to many other materials chemistry based applications. We show that, for surface grafted copper organometallics, and for the study of the selective conversion of methane to methanol using copper ion-exchanged zeolites, the application of focused X-ray beams for operando X-ray spectroscopy is subject to significant challenges if reliable data is to be obtained. We demonstrate how unwanted effects due to the X-rays, which can prevent the study of certain types of reactive system, and/or lead to the derivation of results that are not at all representative of the behavior of the materials in question, manifest. With reference to studies conducted at a beamline that does not focus its X-rays, we then delineate how the total photon throughput and the brilliance of the applied X-rays results in measurements, affects the apparent behavior of copper in the selective conversion of methane to methanol. We show that the use of increasingly brilliant X-ray sources for X-ray spectroscopy can bring with it significant caveats to obtaining valid and quantitative structure-reactivity relationships (QSARS) and kinetics for this class of material. Lastly, through systematic study of these effects we suggest ways to ensure that valuable allocations of X-ray beam time result in measurements that reflect the real nature of the chemistry under study and not that due to other, extraneous, factors.