KN14 | Capturing Functional Nanostructures And Their Interfaces With Neutron Total Scattering

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It is widely recognized in catalysis, fuel cell and battery chemistry, bio- and geochemical processes, and a host of additional functional materials areas that unique properties and characteristics are governed by intricate structural-chemical relationships. Uncovering the identity and role of locally ordered motifs, including those of surface species and interfaces, remains a challenge because experimental tools to observe materials at atomic length-scales, in relevant operating conditions, or within sufficiently fine time scales are limited. We present our efforts to apply and extend neutron total scattering and related probes towards capturing the interplay of crystal chemistry and functionality in nano- and nanostructured materials. Examples include: (1) exploration of internal dipole-dipole ordering in ferroelectric nanocrystals, demonstrating the enhancing effects of cubic particle shape and polar surface termination; (2) investigation of layered manganese oxide structures, where interlayer water molecules, hydrogen bonding, and the nature of vacancies/intercalants strongly impact catalytically and electrochemically active variants; and (3) demonstrated abilities to probe the structure and dynamics of gas-solid interfaces in catalytic materials, where the signatures of interfacial species are enhanced through neutron isotope contrast techniques. These examples improve understanding of technologically and geologically significant materials and highlight a broader theme of our research aimed at extracting crystal structure models from experimental data with the detail needed to guide and validate modern nanoscale theories, and design new and improved functional materials. Current challenges and future opportunities in this arena will be discussed.