Priority Programme

"Material Synthesis near Room Temperature"

SPP 1708

Project Description – Project Proposal

Molecular design and X-ray spectroscopy of & on iron nanocluster catalysts

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Summary of proposal

The aerobic conditions on our planet have enabled the accumulation of oxidized matter whereas reduced chemicals constitute the most valuable energy carriers. Future shortages of energy-rich resources make efficient reductive transformations one of the greatest scientific challenges. This project combines the action of the most abundant transition metal iron in challenging reductive transformations and advanced synchrotron-based characterization techniques. The outcomes of this collaborative effort will have major implications for modern chemical synthesis/catalysis and materials and energy research as well as the application of hard X-ray to understand and improve such systems. Our endeavour capitalizes on the higher reducing power and enhanced sustainability of iron catalysts over noble metal technologies. However, the design of active low-valent Fe catalysts, the realization of new catalytic reactions, and their mechanistic understanding will only be possible through the controlled generation and effective stabilization of reduced Fe species. Major emphasis will be placed on the nature of the interaction between iron(0) nano-particles and surface-active ligand and solvent systems that modulate the stereo-electronic properties of the catalyst. We address various approaches to the bottom-up synthesis of Fe(0) nanoparticles in solution, including. Catalytic reactions of utmost relevance to the manufacture of valuable chemicals and materials will be studied (reductions, hydrogenations,

defunctionalizations etc.). Detailed spectroscopic investigations with hard X-rays aim at understanding the interplay between synthesis parameters and the size, surface properties and oxidation state of the iron nanoparticles and their dynamic changes during the nanoparticle synthesis and catalytic reactions. This collaborative project extends well beyond the realm of chemical synthesis into materials research, spectroscopy and solvent technologies with direct relevance to sustainable production and energy technologies. Our interdisciplinary program provides new sets of reducing iron catalysts, new reduction protocols, and new spectroscopic methods.