Poster Presentation

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Locating Cu in Zeolite SSZ-13 by Synchrotron PXRD Using Maximum Entropy Method

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Efficient elimination of environmentally harmful gaseous NOx compounds from automotive diesel emission remains a challenging task. State-of-the-art zeolites with the chabazite framework containing catalytically active Cu2+ (Cu-SSZ-13) have been commercialized as NOx after-treatment catalysts in diesel-powered vehicles, due to its superior activity, selectivity, and durability.[1] However, to meet current and future legislative demands, continuous improvement is of fundamental interest. Prerequisites for an in depth understanding and further improvements, are detailed complete structural models of the Cu-loaded catalyst. This may be achieved by the use of high resolution synchrotron powder X-ray diffraction (PXRD) and iterative Rietveld analysis and Maximum Entropy Method (MEM). Since the content of Cu2+ is low, a protonated system (H-SSZ-13) and model system with monovalent Ag+ ions (Ag-SSZ-13) are also examined. The protonated and dehydrated H-SSZ-13 shows perfectly empty voids, i.e. no water residue or other non-framework species. The H-SSZ-13 structure is used as the initial model for the MEM calculations. For Ag-SSZ-13 MEM analysis clearly pinpoints the Ag+ ion as being located in the 6-ring shifted into the chabazite cage (Figure 1), consistent with the generally accepted site for Ag+ ions in chabazite and reveals the strength of the iterative Rietveld/MEM analysis. For the more challenging case of Cu-SSZ-13 it was still possible through careful analysis and reasoning to locate two separate positions for the Cu2+ in Cu-SSZ-13 (Figure 1). The B site has been suggested by several other studies, but never confirmed experimentally.[2] This is the most complete structural description of zeolite SSZ-13 with stabilizing and catalytically active Cu2+ ions.[3]

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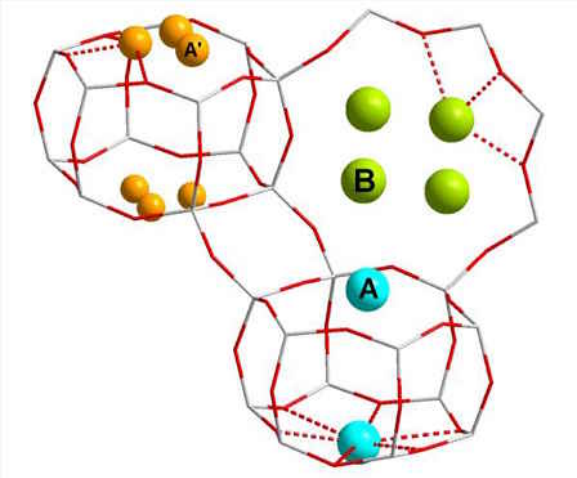

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