# Local structure of nanosized photocatalysts probed by X-ray absorption spectroscopy

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Nanostructured tungstates $CoWO_4$ and $CuWO_4$ are very promising catalytic materials, particularly for photocatalytic oxidation of water. The high catalytic activity of tungstate nanoparticles is partially a result of their extremely small sizes, and, consequently, high surface-to-volume ratio. Thus the properties of such material strongly depend on the atomic structure, which, in turn, can significantly differ from that in the bulk [1].

X-ray absorption spectroscopy is a powerful technique to study the local atomic and electronic structure of nanomaterials. In this study we employ the novel reverse Monte Carlo - evolutionary algorithm (RMC/EA) approach [2] for the analysis of the extended X-ray absorption fine structure (EXAFS) spectra from nanosized (smaller than 2 nm) $CoWO_4$ and $CuWO_4$ powders (Fig. 1). The RMC/EA-EXAFS method and simultaneous analysis of the W $L_3$- and Cu/Co K-edge EXAFS data allowed us for the first time to obtain a 3D structure model of tungstate nanoparticles and to explore in details the effect of size, temperature and transition metal type.

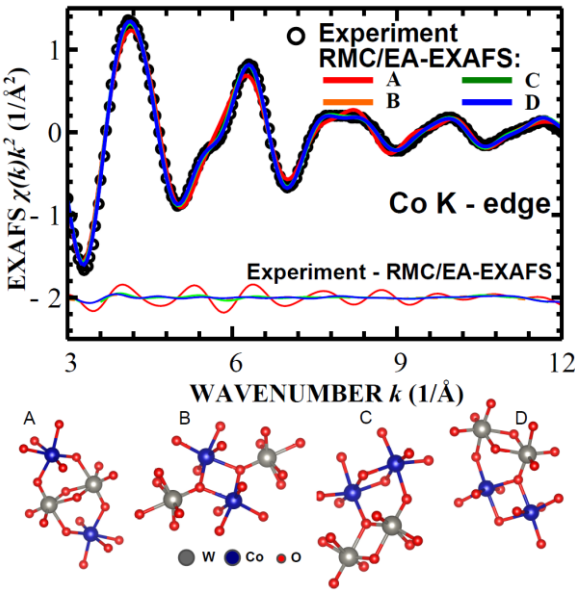


Fig.1 The experimental Co K-edge EXAFS spectrum of nanocrystalline $CoWO_4$ at room temperature (circles) and the results of the RMC/EA simulations starting from four different structure models (A, B, C and D) (solid lines).

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References

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2. J. Timoshenko, A. Kuzmin, J. Purans, J. Phys.: Condens. Matter **26**, 055401 (2014)