Interactions of metal oxide nanoparticles and proteins – structural insights and application perspectives

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Metal oxide nanoparticles are potentially attractive tools for biomedical applications such as bioimaging and drug delivery. This urges experimental studies of their surface interaction with biomolecules, in the first hand, amino acids and proteins. Especially intriguing is the effect of not only shape and size but of chemical nature of the particles on the nature of bonds emerging between them and biomolecules. In present study we isolated, structurally characterized and compared complexes with model molecules glycylglycine and arginine of spherically shaped Keggin POMs $[PM_{12}O_{40}]^{3-}$, M = Mo, W as models for individual nanoparticles ca. 1 nm in size. Surprisingly, structures of the chemically analogous Mo- and W-compounds were not isomorphous, and in case of arginine cations even differed in compositions. The structures of Mo-derivatives are dominated by charge interactions, while for the W-ones, the hydrogen bonding, leading to possible configuration changes in biomolecules, is of prime importance. Keggin POMs appear to be unstable to hydrolysis on strong dilution according to ^{1}H and ^{31}P NMR and electrospray ionization MS data, but are appreciably stabilized, when in complex with a peptide or an amino acid.

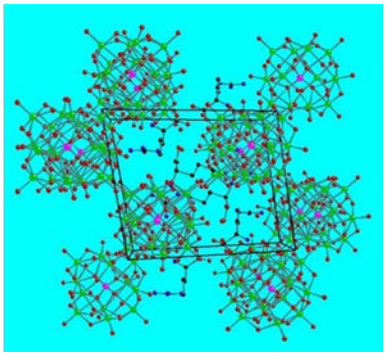

Figure 1. Packing in the structure of $(HGlyGly)_3[PW_{12}O_{40}](H_2O)_6$

[1] K.M. Rominger et al. Eur. *J. Inorg. Chem.* **2019**, *in press*, DOI: 10.1002/ejic.201900611