Design principles for peroxidase-mimicking nanozymes

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Nanozymes, enzyme-like catalytic nanomaterials, are considered to be the next generation of enzyme mimics because they not only overcome natural enzymes' intrinsic limitations, but also possess unique properties in comparison with conventional artificial enzymes. Until now, lots of nanomaterials have been explored to mimic various natural enzymes, such as peroxidase, oxidase, catalase, and hydrolase. Particularly, enormous efforts have been devoted to peroxidase-like nanozymes because of their applications in biomedical diagnosis, bioimaging, anti-biofouling coatings, etc.

While breakthroughs in peroxidase-like nanozymes have been made recently, most studies are based on trial-and-error strategies to identify and synthesize suitable peroxidase mimics. The rational strategies for designing effective nanozymes with peroxidase-like activity will be a major step forward in this important and emerging field, because it requires the identification of predictive descriptors – structural characteristics of the nanomaterials that can be used as proxies for their peroxidase-like activities.

To meet this challenge, Wei and co-workers reported that the efficacy of a descriptor based on the occupancy of antibonding eg orbitals (i.e., eg occupancy) to predict and optimize the peroxidase-like activity of perovskite transition metal oxide (TMO) nanomaterials. They identified a volcano relationship between the occupancy and the catalytic activity: namely, perovskite TMOs with an occupancy of around one and zero (or two) exhibited the highest and lowest peroxidase-like activity,

respectively. The volcano relationship was further rationalized by density functional theory (DFT) calculations. The occupancy descriptor successfully predicted the peroxidase-like activity of binary TMOs with the same octahedral coordination geometries.

This study provides not only a straightforward and predictive activity descriptor for guiding the search for highly active peroxidase mimics but also molecular insights for understanding the mechanisms of the nanozyme catalyzed reactions.

More information: Xiaoyu Wang et al. eg occupancy as an effective descriptor for the catalytic activity of perovskite oxide-based peroxidase mimics, *Nature Communications* (2019). DOI: 10.1038/s41467-019-08657-5

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