Defect-mediated optimal nanoscale magnetic functionalities

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The quest for nanoscale crystals that surpass the performance of a single core is motivated by the design-concept of controlling the spatial distribution of chemical composition within a single motif. In that respect, colloidal magnetic nanocrystals designed for important biomedical applications, [1] such as magnetic hyperthermia treatment of tumours, occasionally require defect-free, large entities (>20 nm) due to their high capacity to dissipate heat in their near vicinity. However, this attribute may come with some drawbacks, including patient discomfort. We combine nanochemistry, detailed characterization and theoretical Monte Carlo considerations to explore the relation of structural defects on the size and shape of iron-oxide nanocrystals and how these couple to magnetic properties relevant to nanobiotechnology [2]. Connecting compositional complexity and nanomagnetism allows us to gain insights on how controlled cation vacancy-induced disorder tailors physical properties, including exploitable thermal energy transfer for small-size magnetic nanocarriers. Unique, synchrotron X-ray total scattering methods attest that size-dependent evolution of the metal-cation valence state, produces pinning defects, which promote favourable magnetic interactions at subcritical sizes (10 nm), and beyond the limitations of finite-size effects alone. The investigation suggests the broader implications of atomic-scale defect control as a design parameter that favours anisotropic properties for optimized nanomaterials, with simultaneous diagnostic and therapeutic functionalities (cf. theranostics).

[1] D. Yoo et al., *Acc. Chem. Res.* **44**, 863, (2011).
[2] A. Lappas et al., *Phys. Rev. X* **9**, 041044 (2019).