Core-selective silver-doping of gold nanoclusters by surface-bound sulphates on colloidal templates: From synthetic mechanism to relaxation dynamics

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Ultra-small luminescent gold nanoclusters (AuNCs) have gained substantial interest owing to their low photobleaching and high biocompatibility. While the substitution of silver for gold at the central core of AuNCs has shown significant augmentation of photoluminescence with enhanced photostability, selective replacement of the central atom by silver is, however, energetically inhibited. Herein, we present a new strategy for *in situ* site-selective Ag-doping exclusively at the central core of AuNCs using sulfonated colloidal surfaces as the templates. This approach exceedingly improves the photoluminescence quantum efficiency of AuNCs by eliminating non-radiative losses in the multi-step relaxation cascade populating the emissive state. Density functional theory predicts the mechanism of specific doping at the central core, endorsing the preferential bonding between Ag^{+} ions and sulphates in water. Finally, we unravel the generic nature of the templating concept to allow core-specific doping of nanoclusters.