Size- and shape-dependent binding of conductive polymer ligands in sintering-free gold nanoparticle hybrid inks for printed electronics

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Functionalization of metallic nanoparticles with conductive polymer ligands enables sintering-free inks that are suitable for inkjet-printed electronics. We prepare colloidally stable hybrid ink that yield conductive structures upon drying by stabilizing gold nanoparticles with a conductive polythiophene ligand [1]. In the dried state, the large, delocalized, π-conjugated system of the polymer improves the inter-particle charge carrier transport [2]. Carrier transport in conductive polymers is dominated by inter-chain and intra-chain hopping processes. Control over the polymers' configuration on the particle surface therefore is crucial for the design of highly conductive materials.

Here, we report on the relation between polymer ligand orientation and the size and shape of the metal core. We investigated polymer binding on spherical and rod-shaped gold nanoparticles by Raman spectroscopy and X-ray photoelectron spectroscopy. The spectroscopic results show that the polymer ligands bind the metal surface both through sulphur in the polymer backbone and through sulphur in the side chains. Size and the shape of the gold core changed the contributions of the different sulphur species. We believe that changes in surface curvature led to different orientations of the polymer chains in the ligand shell. Increasing surface curvature of the metal core favoured the space-demanding "edge-on" binding configuration over the compact "face-on" configuration of the polymer. This caused an "edge-on" to "face-on" transition from spherical to rod-like particles (Fig. 1).

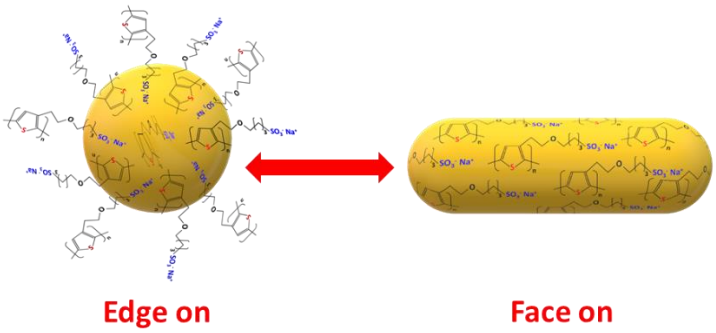

Figure 1. Dominant "edge-on" orientation of the polymer ligand on spherical gold nanoparticles (left) and preferential "face-on" binding on gold nanorods (right).

[1] B. Reiser et al., *Chem. Sci.* **7** (2016), 4190.
[2] T. Minari et al., *Adv. Funct. Mater.* **24** (2014), 4886.

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