Conductive Polymer Shell Formation in Gold–Polythiophene Hybrid Nanoparticles for Sinter-Free Printed Conductors

Muniba S. Bhatti [1,2], Thomas Kister [1] and Tobias Kraus [1,2]

[1] INM-Leibniz Institute for New Materials, Campus D2 2, Saarbrücken, 66123, Germany, [2] Saarland University, Colloid and Interface Chemistry, Saarbrücken, 66123, Germany

muniba.bhatti@leibniz-inm.de

Colloidal metal nanoparticle inks are widely used in printed electronics.[1,2] Many require high-temperature (>150 °C) post-treatments to reduce contact resistance and achieve sufficient electrical conductivity, limiting compatibility with flexible substrates.[3] Conductive ligand shells offer an alternative by enabling charge transport without sintering.[4] However, their formation is complex and strongly influences conductivity.[5,6] This work focuses on the pH-controlled formation of conductive polythiophene shells via ligand exchange and its impact on interfacial properties. We investigate the effect of pH on the exchange of cetyltrimethylammonium bromide (CTAB) on gold nanoparticles (60–75 nm) with the conductive polythiophene poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3KHT), emphasizing the role of polymer conformation. Dynamic and static light scattering (DLS/SLS) and UV–Vis spectroscopy show that pH-dependent conformational changes critically affect colloidal stability and ligand exchange efficiency. At pH < 9, reduced electrostatic repulsion induces aggregation, hindering controlled shell formation. Raman spectroscopy indicates enhanced Au–P3KHT interactions under alkaline conditions, reflected by an increased Au–S/Au–Br peak ratio, consistent with improved polymer binding and surfactant displacement. The addition of 20 mM NaCl further facilitates CTAB removal by screening electrostatic barriers. X-ray photoelectron spectroscopy (XPS) reveals new S2p components at lower binding energies above pH 11, indicating stronger polymer–gold interactions. Preliminary electrical characterization shows enhanced conductivity for samples prepared under alkaline conditions (σ = 6.1–9.5 × 10^4 S m^{-1}), demonstrating suitability for sinter-free conductive inkjet inks.

Keywords:
Hybrid nanoparticles, gold ink, polythiophenes

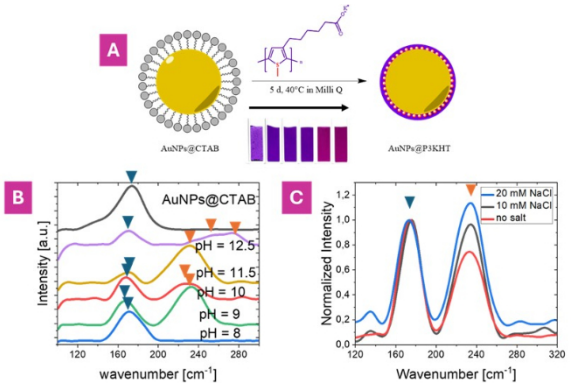

Figure 1: (A) Replacement of CTAB with P3KHT over ligand exchange in Milli Q at various pH. (B) Raman spectra of dry films of AuNPs@P3KHT after ligand exchange in different pH. (C) Raman spectra of AuNPs@P3KHT at pH 10.8 with different salt concentrations.

References:

[1] Benson, C. M. Fung, J. S. Lloyd, D. Deganello, N. A. Smith and K. S. Teng, Nanoscale research letters, 2015, 10, 127.
[2] Deng, X. Zhang, Z. Zhang, Z. Xin and Y. Song, Journal of nanoscience and nanotechnology, 2014, 14, 5114–5119.
[3] J. McClure, Proceedings of the annual technical conference-society of vacuum coaters, 2007, p. 692.
[4] Minari, Y. Kanehara, C. Liu, K. Sakamoto, T. Yasuda, A. Yaguchi, S. Tsukada, K. Kashizaki and M. Kanehara, Advanced Functional Materials, 2014, 24, 4886–4892.
[5] Reiser, L. González-García, I. Kanelidis, J. H. Maurer and T. Kraus, Chemical science, 2016, 7, 4190–4196
[6] K. Backes, L. González-García, A. Holtsch, F. Müller, K. Jacobs and T. Kraus, The Journal of Physical Chemistry Letters, 2020, 11, 10538–10547.