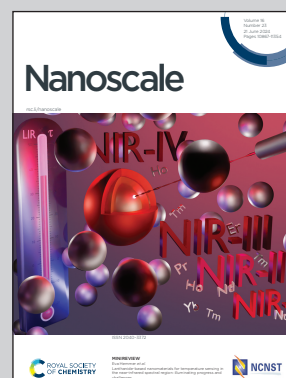


Showcasing research from Professor Mathieu Frenette and Professor Ali Nazemi's laboratory, Department of Chemistry, Université du Québec à Montréal, Québec, Canada.

Insight into the nature of carbon-metal bonding for *N*-heterocyclic carbenes in gold/silver complexes and nanoparticles using DFT-correlated Raman spectroscopy: strong evidence for  $\pi$ -backbonding

*N*-Heterocyclic carbenes (NHCs) are promising ligands for stabilizing metallic complexes, nanostructures, and surfaces. The carbon-metal bond in NHCs crucially affects the material's properties. Raman detection reveals NHC-Au/Ag bond-stretching vibrations inaccessible to standard infrared spectroscopy. Investigating conflicting reports on  $\pi$ -backbonding, we confirm its existence *via* analysis of C=N stretching decrease and EDA-NOCV calculations. NPs exhibit weaker  $\pi$ -backbonding, partially explaining weaker NHC-NP bonds than in metallic complexes.

As featured in:



See Ali Nazemi, Mathieu Frenette *et al.*, *Nanoscale*, 2024, **16**, 11052.