Insight into the Electronic Structure of the Supramolecular Au−Cu and Au−Ag Self-Assembled Complexes from X-Ray Photoelectron and Absorption Spectroscopy

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The recently discovered “rods-in-belt” supramolecular complexes with Au-Cu or Au-Ag cluster cores exhibit self-assembly behavior, have a very unusual structural motif, and what is most important, show remarkable light emitting properties. The electronic and photophysical characteristics of these unique objects can be relatively easy tuned by modifying the ligand (alkynyl and phosphine) environment. Because of these properties the “rods-in-belt” supramolecules could serve as building blocks for next generation electronics, and in particular, for light-emitting devices and in bioimaging applications.

Combining XPS and NEXAFS measurements, we disentangle the structure of occupied and unoccupied electronic states near the Fermi level for both Au-Cu and Au-Ag families of these supramolecules. The detected that difference of the HOMO-LUMO gap for Au-Cu and Au-Ag complexes nicely correlates with the optical absorption of the discussed compounds. It was also revealed that with increasing size complexes become more sensitive to X-ray damage.

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