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Host-Guest Chemistry in Boron Nitride Nanotubes: Interactions with Polyoxometalates and Mechanism of Encapsulation

Boron nitride nanotubes (BNNTs) are an emerging class of molecular container offering new functionalities and possibilities for studying molecules at the nanoscale. Herein, BNNTs are demonstrated as highly effective nanocontainers for polyoxometalate (POM) molecules. The encapsulation of POMs within BNNTs occurs spontaneously at room temperature from an aqueous solution, leading to the self-assembly of a POM@BNNT host-guest system. Analysis of the interactions between the host-nanotube and guest-molecule indicate that Lewis acid-base interactions between W=O groups of the POM (base) and B-atoms of the BNNT lattice (acid) likely play a major role in driving POM encapsulation, with photoactivated electron transfer from BNNTs to POMs in solution also contributing to the process. The transparent nature of the BNNT nanocontainer allows extensive investigation of the guest-molecules by photoluminescence, Raman, UV-vis absorption, and EPR spectroscopies. These studies revealed considerable energy and electron transfer processes between BNNTs and POMs, likely mediated via defect energy states of the BNNTs and resulting in the quenching of BNNT photoluminescence at room temperature, the emergence of new photoluminescence emissions at cryogenic temperatures (<100 K), a photochromic response, and paramagnetic signals from guest-POMs. These phenomena offer a fresh perspective on host-guest interactions at the nanoscale and open pathways for harvesting the functional properties of these hybrid systems.

References

[1] Jack W. Jordan, Alexander I. Chernov, Graham A. Rance, E. Stephen Davies, Anabel E. Lanterna, Jesum Alves Fernandes, Alexander Grüneis, Quentin Ramasse, Graham N. Newton, Andrei N. Khlobystov, Journal of the American Chemical Society, 145 (2023) 1206-1215

Figures

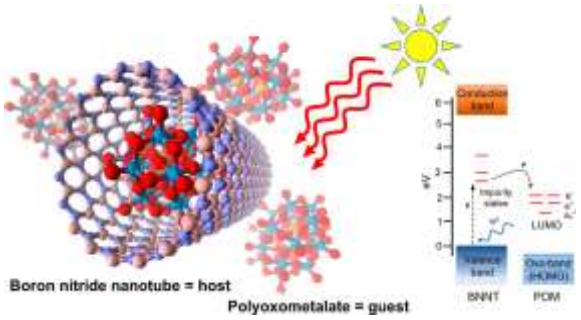

Figure 1: Photoactivated electron transfer from BNNTs to POMs plays a major role in driving POM encapsulation.