

On the cation?? capabilities of small all sp²-carbon host structures. Evaluation of [6.8]3cyclacene from relativistic DFT calculations

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Cation?? interactions are noncovalent forces with essential roles in the stability of protein structures, molecular recognition, and host?guest chemistry. In this work, we discuss the formation of cation?? complexes involving one of the smallest characterized nanobelts to date, given [6.8]3cyclacene, by using relativistic DFT-D calculations. Such nanobelt exhibits a noteworthy all-sp² carbon backbone, leading to a rigid and confined host framework. Our results reveal that the inclusion of representative cations, such as Ag⁺ and Sn²⁺, appears to be plausible, revealing that it is feasible to obtain these compounds experimentally. Such systems involves two contrasting coordination modes, where the Ag⁺ cation remains coordinated in the upper face of the nanobelt, whereas the Sn²⁺ is able to be located at the center of the structure. In addition, the coordination of isoelectronic Cd²⁺ and In⁺ was also discussed. Moreover, the bonding characteristics of the resulting cation?? interaction show that the ?-orbitals from the nanobelt 1 are able to moderate the charge transfer, according to the selected cation, which can be seen as an interesting strategy to tune the amount of charge of the ?-backbone in nanobelts. We envisage that the use of more rigid host in the formation of cation?? interactions will be beneficial to gain a better understanding about the metal coordination and also to tune the capabilities of related nanobelts or nanotubes sections. © 2018 Wiley Periodicals, Inc.

bonding

cation??

DFT

EDA-NOCV

host

Bonding

Charge transfer

Chemical bonds

Nanobelts

Yarn

Bonding characteristics

Carbon backbone

Coordination modes

EDA-NOCV

host

Metal coordination

Pi interactions

Protein structures

Positive ions