Triangular X_3 Halogen-Bonded Synthons at Play - Insights From Computer Simulations

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The recent decades have witnessed on-surface synthesis (OSS) of diverse molecular architectures unattainable by classical methods of wet chemistry. Among them, especially interesting are surface-supported networks stabilized by X_3 halogen-bonded synthons [1]. To date, numerous ramified building blocks with aromatic backbones have been synthesized and exploited as bridging linkers of diverse homoporous overlayers cemented by triangular halogen–bonded motifs [2,3]. However, much less attention was paid to similar heteroporous architectures comprising mixed halogenated molecules with different symmetries so far. Therefore, in this communication, we present our recent theoretical findings on the bottom-up formation of hierarchically organized openwork co-crystals sustained by anisotropic halogen–bonded motifs on solid surfaces (Figure 1) [4]. The results of our predictive computer simulations could be especially valuable for the scanning tunneling microscopy (STM) experimentalists interested in the bottom-up fabrication of novel nanomaterials where directional halogen–halogen intermolecular interactions play a decisive role. This work was supported by the National Science Centre, Poland research grant: 2018/31/D/ST4/01443, SONATA 14.

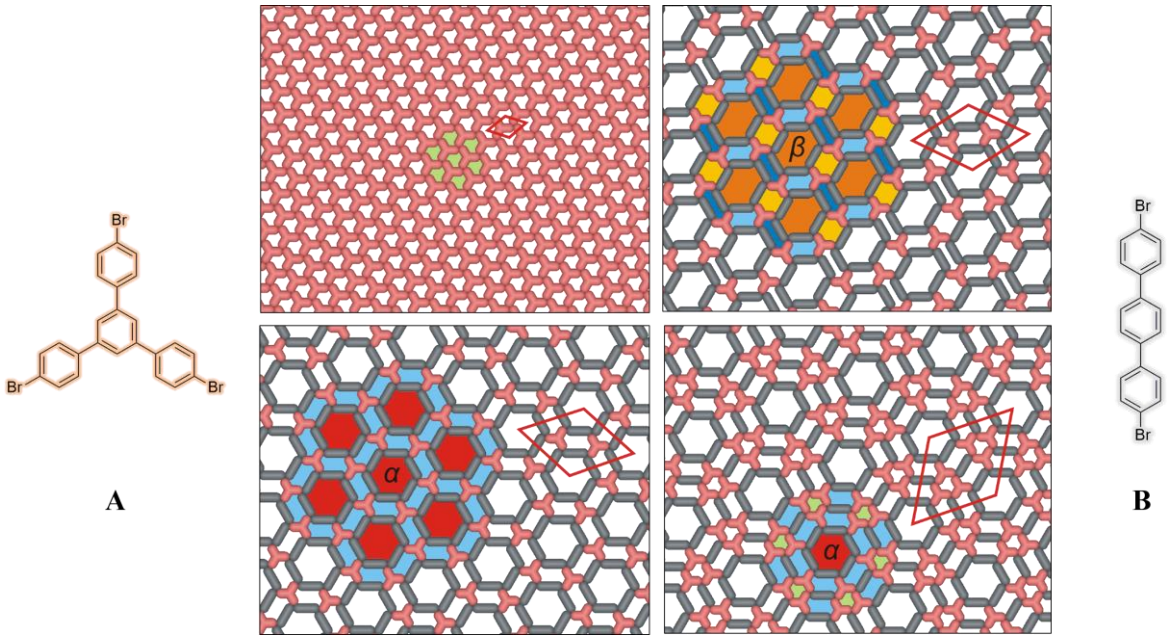

Fig. 1. Exemplary two-dimensional (2D) polymorphic networks cemented by X_3 halogen bonds between star-shaped (**A**) and rod-like molecules (**B**) mixed in different stoichiometric ratios. Computer Monte Carlo (MC) simulations results.

[1] J. Shang, Y. Wang, M. Chen, J. Dai, X. Zhou, J. Kuttner, G. Hilt, X. Shao, J. M. Gottfried, Nature Chemistry, **7**, 389 (2015)
[2] H. Wang, J. Hu, Z. Liang, H. Zhang, C. Huang, L. Xie, Z. Jiang, H. Huang, F. Song, Nanoscale Advances, **5**, 1368 (2023)
[3] Q. Fan, L. Liu, J. Dai, T. Wang, H. Ju, J. Zhao, J. Kuttner, G. Hilt, J. M. Gottfried, J. Zhu, ACS Nano, **12**, 2267 (2018)
[4] D. Nieckarz (unpublished results)