Escape from Molecular Flatland: Frustration, Adaptation, and Cooperation

Dongwhan Lee

Department of Chemistry, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea
dongwhan@snu.ac.kr

Structure begets function. Novel functions emerge from novel structures, either by rational molecular design (as we often claim retrospectively even without guilt) or by sheer serendipity (although we ordinarily do not disclose). For some time now, my research group has been exploring the chemistry of triazole-fused polyaromatics as conformationally well-defined *turn motifs* for spontaneously folding π-conjugated molecules and self-assembling macrocycles.

What new properties would emerge if close π-π contacts between large and flat aromatic surfaces are intentionally thwarted? This open-ended question prompted our recent ventures into the chemistry of (i) porous crystals displaying cavity-changing motions, (ii) hydrophobic collapse of polycationic fluorophores, (iii) allosteric gating of canopied container molecules, and (iv) hierarchical folding of cation-responsive molecular tweezers. This presentation will discuss key design principles, synthetic implementations, and functional consequences of the steric and electronic frustration that is endured (and also exploited) by non-stackable triazoliptycenes, isobenzimidazoles, and peralkylated benzenes.

