Editorial

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Special Issue: Self-Assembled Molecules/Materials

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Research on self-assembled molecules and materials formed by non-covalent interaction/s has bloomed in last two decades due to their diverse shapes, sizes and applications. Among all the non-covalent interactions, H-bond and metal-ligand coordination interactions have been preferred choices due to their strong directional nature that helps in designing the target structures. Due to dynamic reversible nature of the self-assembly, it undergoes several self-correction steps. Finally, the thermodynamically stable structure prevails over the other possible kinetically controlled structures and thus becomes devoid of any structural defects. Further, with the possibility of attaching suitable functional groups in the building blocks, these materials have been designed for various applications in biomedical, catalysis, switchable materials, chiral recognition/separation, etc. Despite enormous research done in this area, design and synthesis of more complex structures selectively with new functions is still a challenging research problem that many researchers are trying to address. The current theme issue comprises of one review and nine personal accounts discussing the various aspects and challenges in the design and synthesis of self-assembled molecules and materials of diverse structures and functions.

Ki-Whan Chi and co-workers discuss their unique template-free approach for the synthesis of non-trivial, coordination, and non-covalent interaction-driven self-assembled macrocycles/catenanes. Hydrogen bonded dinucleoside based macrocycles have been discussed by David Gonzalez-Rodriguez and co-workers. On the other hand, Sun et al. presents di- and polynuclear metal-cluster-based coordination cages and describes the benefit of blending the properties of both cage and metal clusters in tuning the performance of the final assemblies in sensing, catalysis, and host-guest chemistry. Bruno Therrien and co-authors discuss their excellent efforts in the field of arene-ruthenium assemblies and their biological applications in drug delivery, DNA interactions, photodynamic therapy, and imaging. A brief account by Schmittel et al. describes the emerging field of molecular cybernetics and highlights their enormous contributions in this area in last few years. Luminescent materials are of specific importance in terms of sensing application. Lescop et al. presents here luminescent and electronic properties of Cu (I) based supramolecular systems, in which the photophysical behavior of Cu(I)-luminophores has been explored. Further, Keisuke Umakoshi and co-authors discuss the luminescent properties of heteronuclear complexes involving heterometallic metal-metal interactions. They also elaborate here interesting encapsulation-induced emission enhancement (EIEE) behaviour, based on emissive host-guest systems consisting of metal complexes and hydrogen-bonded capsules. Apart from this, another class of materials that has recently attracted considerable attention is the covalent organic discrete molecules. They follow dynamic covalent chemistry as their formation tool, and comprise interesting structures like macrocycles, cages, molecular knots, catenanes, rotaxanes, etc. Solution processability is one of the important aspects of self-assembled systems, which makes them inimitable from the extended frameworks. Michael Mastalerz and co-workers discuss their exclusive approaches of suppressing the long-range packing of aromatic molecules and rather driving them to form solution-processable polyaromatic compounds based on triptycene backbone. Finally, a brief account of how the theoretical simulations and experimental data go hand in hand has been shown by Hiraoka and co-workers. As we all know that theoretical simulations are wonderful tools to understand and predict the synthetic conditions and pathways for the generation of rather seemingly impossible architectures. Here, they have discussed their self-developed experimental and numerical approach QASAP (quantitative analysis of self-assembly process) and NASAP (numerical analysis of self-assembly

process), respectively, in the investigation of coordination assemblies based on Pd(II)-metal center. The review by Malaichamy and co-workers describes newly evolving spacer based metallo-architectures including their functions.

I would like to express my sincere gratitude to all the contributing authors and reviewers for making this issue possible and I hope that the readers will enjoy reading this excellent issue on self-assembled molecules and materials.

Partha Sarathi Mukherjee, Guest Editor