COMPUTATIONAL STUDY OF HETEROCIRCULENES:

OXIFLOWERS, SULFLOWERS, PYRROFLOWERS, AND PHOSPHOFLOWER

FROM 2D MOLECULES TO 3D GIANT COVALENT FRAMEWORK

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This is a presentation about new findings in the electronic properties of four circulene classes Oxiflowers, Sulflowers, Pyrroflowers, and Phosphoflower. In Oxiflower and Sulfower classes, which are related to several structural parameters. Specifically, it is found that correlations between the HOMO-LUMO gap and some electronic properties of these circulenes are opposite to those of linear conjugated structures. Moreover, a number of new hybrid molecules, called an Oxisulflower, is proposed to be a potential structure for synthesizing as Sulflower. Also, a brand-new descriptor, namely, the "degree of non-planarity", is evaluated with excellent correlations with the HOMO-LUMO gap of molecules in Oxiflower and Sulflower classes. The correlations have also shown that the steric characteristic of a structure can be controlled to modulate its band gap for studying the prediction science of the electronic properties in developing organic semiconductors. From the achievement of Oxiflowers and Sulflowers, two new classes are suggested Pyrroflowers, and Phosphoflower, which are also studied at the same progress as two former sample classes. From four main classes of circulenes, a new type of flower, called SILKY flower, has been created by mixing them together. Interestingly, a brand-new type of giant covalent framework has been designed by connecting the SILKY flowers via saturated carbon chains, converting the 2D flower to 3D structures. This series is believed to open a breakthrough in studying heterocirculene structures with large numbers of fused rings to giant covalent clusters.