Buckybowls: A Theoretical Point of View

TCI SEMINAR

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3:00 p.m. Room 9341

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Open geodesic polyaromatic hydrocarbons mapping onto the surfaces of fullerenes (and therefore often referred to as buckybowls or fullerene fragments) represent a unique class of non-planar p-conjugated molecules. In contrast to the Nobel Prize winning graphene, they possess built-in curvature and strain and have two non-equivalent p-surfaces, *concave* and *convex*, that are readily accessible. This class of bowl- and basket-shaped polyarenes is growing rapidly. Their potential applications range from rational design of fullerenes, nanotubes and their endohedral compounds to supramolecular architectures, for they can act as molecular clips and tweezers or even potential material for new-type Li-batteries. Due to extreme sensitivity of such systems, theoretical modeling seems to be very useful and, sometimes, the only possible tool in studying of their properties. In my talk, I would like to show how the reactivity and properties of unusual open-geodesic polyaromatic organic molecules, in their reaction with different organic, organometallic and inorganic species, can be specifically tuned with help of theoretical modeling. The predictive power of calculations can be used here to create new molecules and/or tune properties of already know systems, in close interaction with experiment. The future research directions will be briefly outlined.

Theoretical Chemistry Institute Seminar Series