Cross Fertilization of Mathematical & Computational Chemistry: Combinatorics, graph Theory, Bioinformatics

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The talk will exemplify exciting applications of combinatorics, graph theory based algorithms to a number of scientific disciplines, particularly in fullerene chemistry and computational biology. Enumerative combinatorics and algorithms find numerous applications to (1) enumeration of structures of molecules (2) three dimensional cages called fullerenes discovery of which led to the Nobel Prize (3) Nuclear spin statistics and spectroscopy. Cross fertilization of graph theory with chemistry and biology seems to provide an exciting fertile ground for interdisciplinary research in bioinformatics, predictive toxicology, molecular and drug design. Examples of applications from each of these fields will be provided and would include DNA algorithm and graph theoretical characterization of proteomics and genomics.