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Exactly Solvable Models in Quantum Mechanics, Mathematical Physics, Quantum Chemical Calculations

The principal investigation theme in our laboratory is the development of exact analytical solutions to Schrödinger equations for various quantum mechanical problems. The most important of these problems is the explication of analytical structure of the helium ground-state wave functions (one of its component of homogeneity 2 is shown in Figure 1). The helium wave function constitutes the simplest case of an explicitly correlated wave function and can serve as a new paradigm for building novel accurate quantum chemical approaches. Another research direction in our lab is the theory of ZZ polynomials of benzenoids, which can be conveniently used for defining various topological descriptors of these systems. In Figure 2 we show the local aromaticity of hexagonal graphene flakes computed using ZZ polynomials (right) and NMR (left). Our group often assists in the interpretation and assessment of experimental measurements with accurate quantum chemical calculations (Figures 3 and 4).

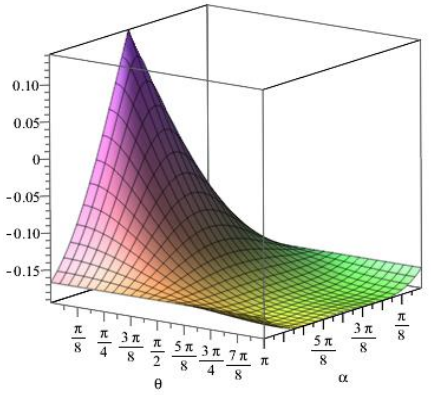
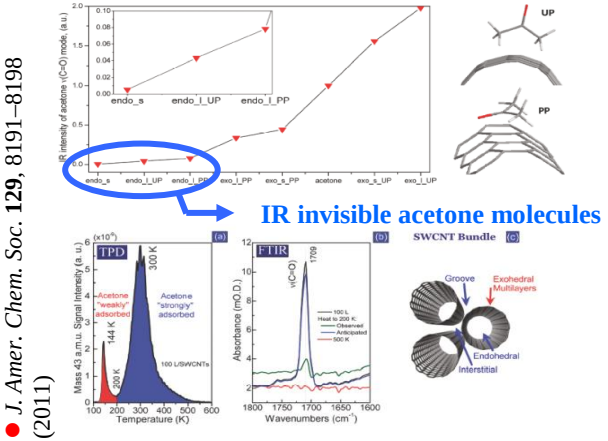


Figure 1

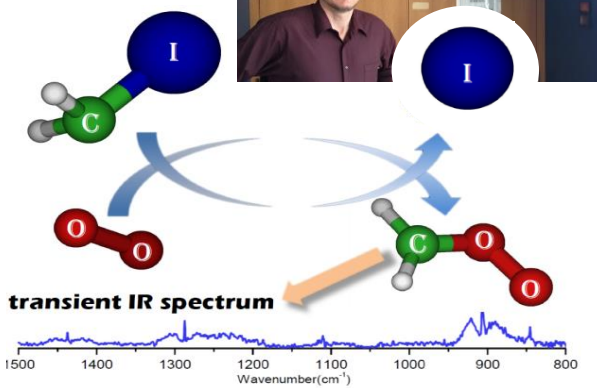
Molecules encapsulated in CNTs are IR invisible



● *J. Amer. Chem. Soc.* **129**, 8191–8198 (2011)

Figure 4

Theoretical calculations permit identification of Criegee intermediates



● *Science* **340**, 174–176 (2013)
● *Nature Comm.* **6**, 7012 (2015)

Figure 3

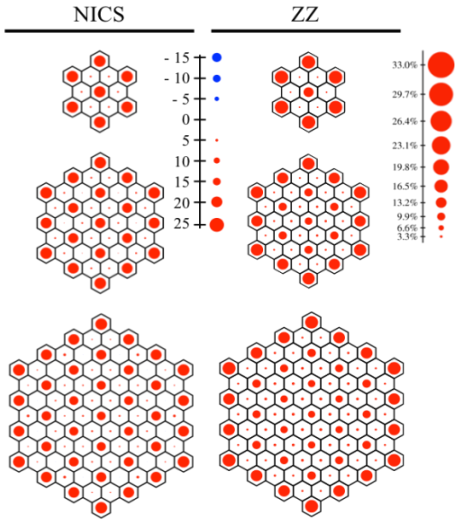


Figure 2