Application of multireference theory: from the photodynamics of nucleobases to graphene multiradical structures

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The photodynamics of DNA and its constituent nucleobases is a highly interesting topic but represents also extremely challenging computational problems because of the necessity of calculating excited state surfaces and their nonadiabatic coupling. In this talk photodynamical simulations based on the COLUMBUS and NEWTON-X programs will be presented showing explicitly the structural and dynamics features of the decay properties of nucleobases in vacuo and with embedding in a DNA environment. As second fascinating topic, the amazing multiradical character of one- and two dimensional graphene flakes will be discussed by means of appropriate multireference calculations on polyacenes and periacenes.