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Functionalization of Carbon Materials by 1,3-Dipolar Cycloadditions

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The reactions of a series of twenty-four different 1,3 dipoles ranging in reactivity from very unreactive, such as nitroalkanes and SO_2, through highly reactive, like ozone and carbonyl ylides, have been studied with high accuracy quantum mechanical methods for small dipolarophiles. The distortion/interaction model and molecular dynamics simulations provide detailed insights into the origins of reactivity differences and the detailed mechanisms of these reactions. The 1,3-dipolar cycloadditions of these species with aromatic carbon materials have been studied both for mechanistic interest and to assess the potential of these reactions for functionalization of fullerenes, nanotubes and graphene for potential electronics applications.