## **DEFECT STRUCTURES IN GRAPHENE MODELS**

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Graphene consists of one single sheet of graphite constructed from a one-atom-thick planar layer of sp<sup>2</sup>-bonded carbon atoms. In this regard, graphene can be referred to as an infinite polycyclic aromatic hydrocarbon (PAH). Recent measurements of its mechanical and electronic properties reveal interesting properties for this nanoscale material. Graphene acts as a semi-metal or zero-gap semiconductor with a remarkably high electron mobility at room temperature. Owing to these features, it represents a very prospective material for nanoelectronics. Nonetheless, it should be noted that the outstanding properties mentioned are only true for the case of pristine graphene. Imperfections of the crystal lattice, such as topological defects, vacancies and substitution atoms have a pronounced effect on them. Therefore, it is crucial to investigate such defect structures in more detail.

In the present work, several defect structures in graphene models (e.g. pyrene, coronene) have been computed by means of high-level quantum chemical methods including perturbation and density functional theory. The first part of this study is dedicated to the interaction between the graphene surface and monovalent alkali metal cations. Beyond that, a detailed investigation on protonation is carried out. Energy minima and transition-state structures are determined and the thermodynamic properties of formation calculated. In the second part of this investigation, defect structures have been studied regarding both the topological (Stone-Wales) defect and vacancies. Aside from that, edge effects have been accounted for as well. Their chemical functionalization with and without an accompanying bond breaking is discussed.