INTERACTION OF PYRENE LIGANDS WITH NEAT AND DEFECTIVE TWO DIMENSIONAL MATERIALS: A FIRST PRINCIPLES STUDY

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Ever since the discovery of graphene [1], scientific communities are in search of other two dimensional (2D) materials which possess unique properties. Due to its semimetallic nature, graphene cannot be accommodated in the list of efficient materials for manufacturing electronic devices. In this regard, many heterogeneous and flat 2D materials with finite band gap have been found which includes nitrides, oxides, and carbides sheets of various elements in the periodic table [2]. For instance, boron nitride (BN), zinc oxide (ZnO), silicon carbide (SiC) and other similar 2D materials with honey comb structure have optimum band gap for various applications.

Recently, our research group has used pyrene based tetratopic ligands (PTL) for functionalizing ZnO nanorods for sensing volatile organic compounds under visible light [3]. Carboxyl groups (COOH) in PTLs are found to be assisting not only for anchoring PTL onto the ZnO, but also it is the efficient site for VOCs adsorption. In this study, graphene and other flat 2D materials of BN, ZnO and SiC are functionalized with ten different pyrene based ligands with various functional groups. The minimum energy structures of the ligands are obtained using molecular dynamics, followed by optimization to their ground states. Similarly, neat and defective graphene, BN, ZnO and SiC sheets are optimized. Single and di-vacancies are introduced in all the 2D sheets. The results of individual 2D functionalized system are being compared and degree of affinity of pyrene ligands towards 2D sheets will be reported. The vacancies are introduced because they are charge rich sites [4]. Hence, they will affect binding tendency of ligands too. Overall, this study will be projected to understand the chemistry of polyaromatic ligands with 2D materials and their usefulness in electronic, optoelectronic, sensing and other exotic applications.

Keywords: Two dimensional materials, Pyrene based ligands, Density functional theory

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