"Nanochemistry and biotechnology"

Anticancer drug carrier properties of Silicene

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Cisplatin, as an important antitumor agent, is currently among the most widely used agents in the chemotherapy of cancer.[1] Due to its side effects and lack of recognizing cancer cell accurately, effective use of cisplatin are hindered[2-4]. However, drug-targeting delivery system enables a stronger drug to be used effectively. The task of carrying the drug can be taken over by nanomaterials. Two-dimensional (2D) materials have been of great interest for various physical properties since the mechanical exfoliation of graphene from graphite[5]. Among these novel 2D honeycomb materials, silicene, with stable buckled honeycomb structures is attractive[6]. Silicene is, in analogy with graphene, predicted to have a band structure forming a Dirac cone with the apex at the Fermi level. One important demarcation is a buckled formation in silicene. This is due to sp^3 and sp^2 hybridization rather than only sp^2 hybridization. This feature leads to a few prominent differences in the properties of silicene[7]. To date, a wide range of potential applications of silicene have been proposed in various field such as spintronics, FETs, hydrogen storage and sensing devices.[8-11] Nevertheless, using silicene as a drug carrier has not been given the attention it deserves. Thus, theoretical study based on Density Functional Theory (DFT) with dispersion correction is carried out to investigate the adsorption geometry, adsorption energy and electronic band structure of Cisplatin/Silicene composite system. It is also shown that how modify structural and electronic properties of cisplatin on silicene by applied charging.

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