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Carborane-wheeled nanocar moving on graphene/graphyne surfaces: van der Waals corrected density functional theory study

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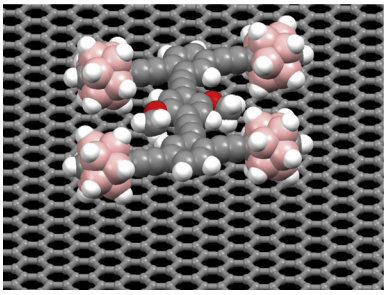
HIGHLIGHTS

- *First-principles* vdW-DF calculations were used to investigate the nanocar motion on graphene/graphyne substrate.
- Two different types of nanocar wheel movement (slipping and slithering) is considered.
- The accuracy of this method is validated by experimental results and the MP2 level of theory.
- *First-principles* molecular dynamics simulation is also used to consider the type of nanocar movement on the substrate.

GRAPHICAL ABSTRACT



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ABSTRACT

Investigations of nanocar motion on one-dimensional substrate surfaces provide an important contribution to the practical goal of designing nanoscale transporters. As a preliminary step toward modeling the dynamics of these species, *first-principles* vdW-DF calculations were performed to investigate the interaction between the nanocar and the graphene/graphyne surface. The accuracy of this method is validated by experimental results and the MP2 level of theory. The results obtained reveal that the nanocar would require at least −71.39 and −18.33 kJ mol^{-1} to activate its movement on the graphene and graphyne surfaces, respectively. *First-principles* molecular dynamics simulations show that the nanocar moved on the substrate without additional external factors under ambient conditions. The nanocar displays a tendency toward slipping on the graphyne surface within 2 ps of simulation time movement. These findings provide insights that will facilitate the coherent design and control of surface-operational molecular machines and a realistic benchmark for the nanocar's movement mechanism.

1. Introduction

Recent efforts have been devoted to the synthesis of nanocars that can perform specific tasks at the molecular level and, ultimately, construct molecular assemblies using a bottom–up approach [1–6]. Nanocars, including molecular motors, are nanostructures that convert electromagnetic energy into mechanical motion [7]. The electromagnetic energy may take various forms, including light, thermal, and electron beams, e.g., nanocars that move simply by heating the substrate. The first nanocar was synthesized by Tour's research group at Rice University in 2005 [8] and consisted of a chassis, four freely rotating axles made of well-

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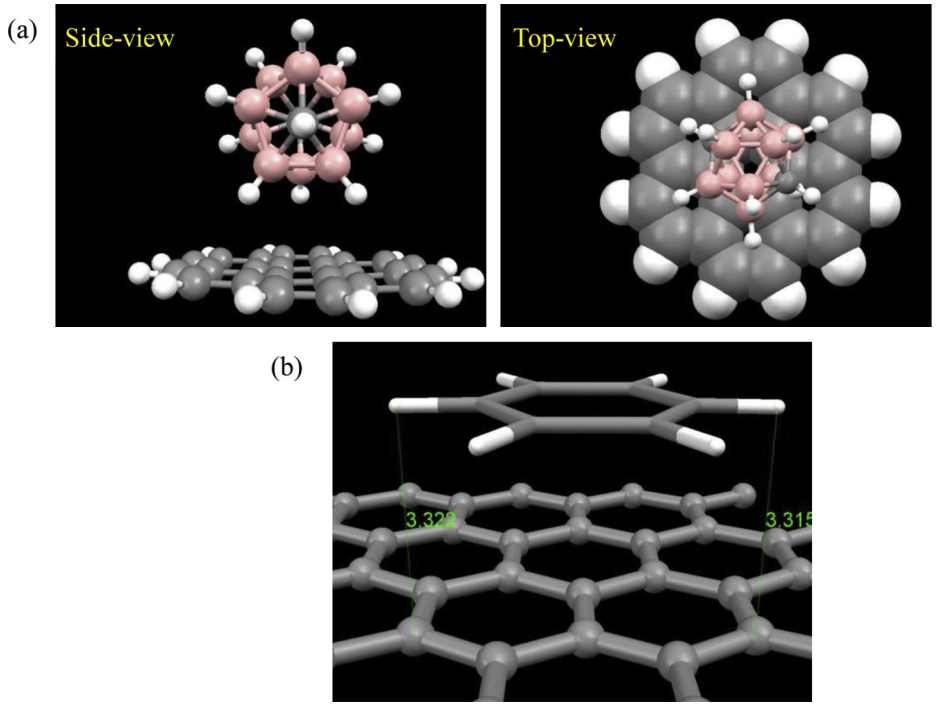

Fig. 1. Schematic representation of (a) a single carborane wheel on the surface of the graphene cluster (coronene), (b) a benzene molecule adsorbed on the graphene surface.

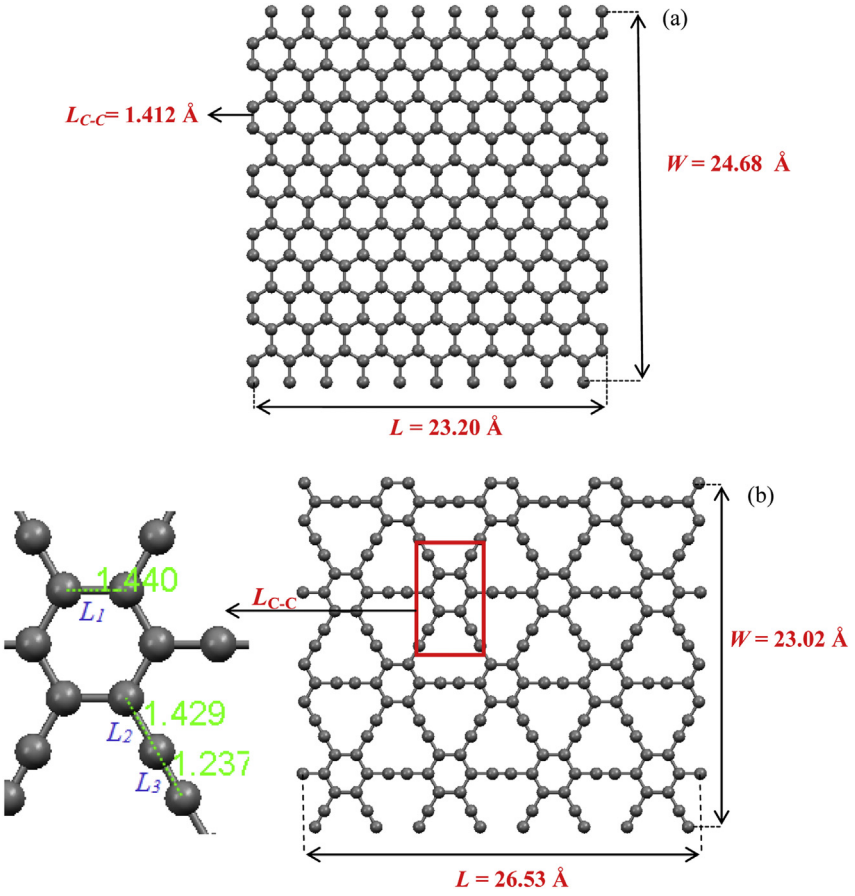

Fig. 2. Optimized structures and geometric parameters, including length (L), width (W), and C–C bond length (L_{C-C}) of (a) graphene and (b) graphyne.