Title

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Abstract

1 Introduction

First synthesized in 2004[9], graphene has since experienced an explosive growth in interest[12]. For pristine graphene, it's interactions with other particles are mainly due to Van der Waals forces and $\pi - \pi$ stacking.[18] As pristine graphene is chemically inert[4] a classical description of it is expected to suffice in simulations. Multiple molecular dynamics studies on the interactions between proteins and carbon based nanoparticles (CBNs) –such as graphene– have been published[1–3,5,6,8,11,16–18]

2 Methods

2.1 Free Energy Methods

2.1.1 Umbrella Sampling

2.1.2 Well-Tempered Multiple Walker Metadynamics

2.2 Molecular Dynamics Simulation

MD simulations were performed using the GROMOS11[13,15] and the NAMD 2.14 simulation packages[10]. Details of the simulations will be presented separately for each program.

2.2.1 GROMOS

The SHAKE algorithm[14] was employed to constrain all bonds to their reference values with a relative tolerance of 10^{-4}, allowing for a time-step of 2 fs using the leapfrog algorithm[7].

2.2.2 NAMD

3 Results

3.1 Adsorption Free Energy

3.2 Adsorption Entropy

3.3 Adsorption Energy

3.4 Diffusion

4 Conclusions

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