Thermodynamic characterization of the adsorption of amino acids onto pristine graphene and graphene oxide

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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 Umbrella Sampling

2.2 Well Tempered Multiple Walk Metadynamics

2.3 Molecular Dynamics Simulation

2.4 Quantum Mechanics / Molecular Mechanics

3 Results

3.1 Adsorption Free Energy

3.2 Adsorption Entropy

3.3 Adsorption Energy

3.4 Diffusion

4 Conclusions

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