

## Accepted Manuscript

Title: The molecular understanding of interfacial interactions of functionalized graphene and chitosan

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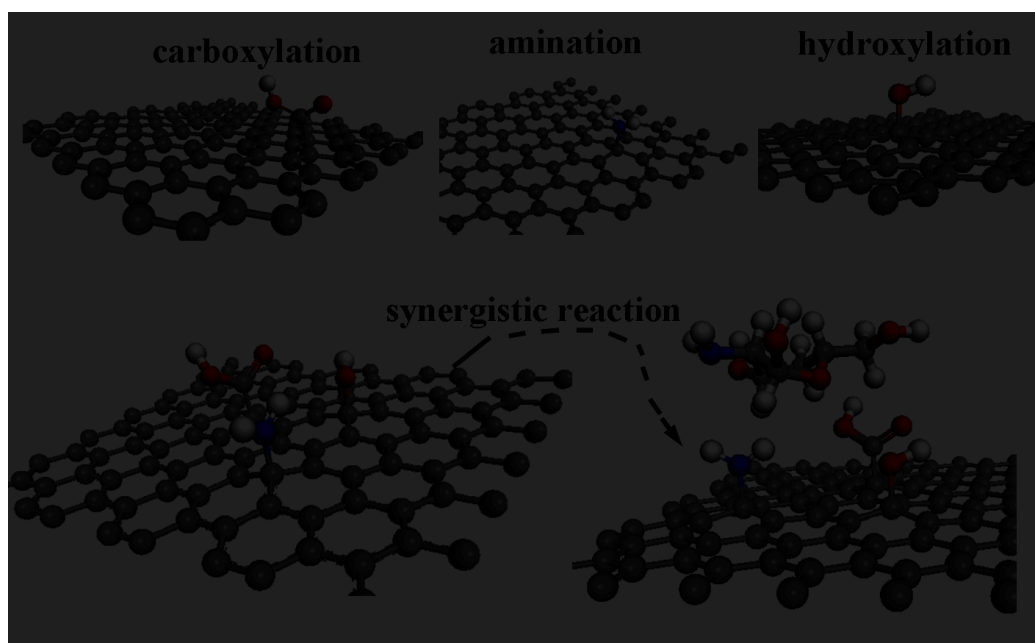
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The type of the functional groups can be used to modulating interactions between graphene sheet and chitosan.

### Highlights

- Investigate interfacial interactions between chitosan and functionalized graphene by DFT
- Observe covalent linkages between COOH-modified graphene and chitosan units
- Multi-functionalized graphene regulates the interfacial interactions with chitosan
- It is useful for guiding the preparation of graphene/chitosan composites

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