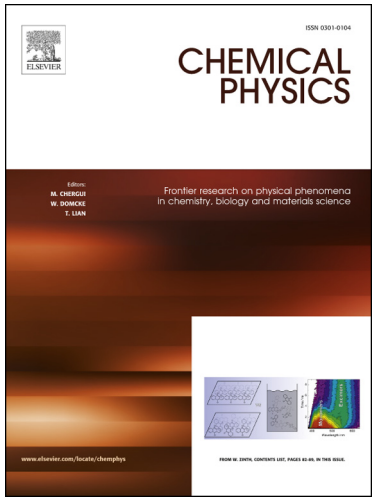


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PII: S0301-0104(16)30147-1
DOI: http://dx.doi.org/10.1016/j.chemphys.2016.05.004
Reference: CHEMPH 9548

To appear in: *Chemical Physics*

Please cite this article as: B. Bhattacharya, U. Sarkar, Graphyne – graphene (nitride) heterostructure as nanocapacitor, *Chemical Physics* (2016), doi: http://dx.doi.org/10.1016/j.chemphys.2016.05.004

# Graphyne – graphene (nitride) heterostructure as nanocapacitor

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## Abstract

A nanoscale capacitor composed of heterostructure derived from finite size graphyne flake and graphene (nitride) flake has been proposed and investigated using density functional theory (DFT). The exothermic nature of formation process of these heterostructures implies their stability. Significant charge transfer between two flakes generates permanent dipole in this heterostructures. The amount of charge transfer is tunable under the application of external electric field which enhances their applicability in electronics. We have specifically focused on the capacitive properties of different heterostructure composed of graphyne flake and graphene (nitride) flake*, i.e.*, graphyne/graphene, graphyne/h-BN, graphyne/AlN, graphyne/GaN. The charge stored by each flake, energy storage, and capacitance are switchable under external electric field. Thus, our modeled heterostructures are a good candidate as nanoscale capacitor and can be used in nanocircuit. We found that the charge stored by each flake, energy storage, and capacitance value are highest for graphyne/GaN heterostructures.

***Keywords:*** Finite size graphyne flake; heterostructures; charge transfer; energy storage; nanocapacitor