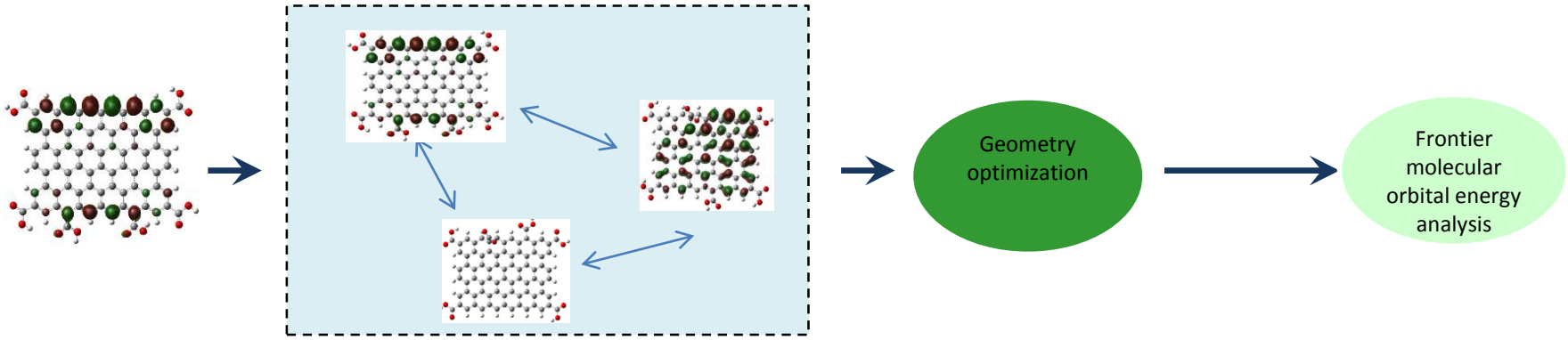
Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Workflow materials models: template 3

DFT calculation



A 28-ring structure model consisting of 78 C atoms and 24 H atoms was selected for simulating the graphene sheet.

According to the ratio of O/C in G-COOH and N/C in G-NH_2, the numbers of functional groups on the surface were calculated to be approximately 6 for both -COOH and -NH_2

Geometry optimization and frontier molecular orbital energy analysis were performed in water at the B3LYP level with the 3-21G basis set using the Gaussian 09 (D.01) simulation package