This dataset contains optimised atomic structures of phosphate species (H3PO4, H2PO4-, HPO42-, PO43-) adsorbed on pristine, curved and oxygenated graphene. The data are the CONTCAR files (output coordinates) produced by density functional calculations using VASP software.

File naming system: {P}-{G}.vasp

Where {P} is the phosphate species (PO4, HPO4, H2PO4, H3PO4) and {G} is the pristine or functionalised graphene species (G, GC-arm, GC-zig, GV, GV-O, GO-epo, GOH-ortho, GOH-ortho2, GOH-para).

A detailed description and discussion of the data, including methodology, can be found in the following peer-reviewed article: Yong, X. et al, ACS Appl. Nano Mater. (2023) 10.1021/acsanm.3c04147. The work was supported by the Natural Environment Research Council (Grant NE/T010924/1).