Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Ab Initio characterization of N doped T-graphene and its application as anode material for Na ion rechargeable batteries

Neha Yadav and T. J. Dhilip Kumar*

Quantum Dynamics Lab, Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar 140001, India

S1: The plot of the energy vs cut-off value for the optimization of E_{cut} is as follows:

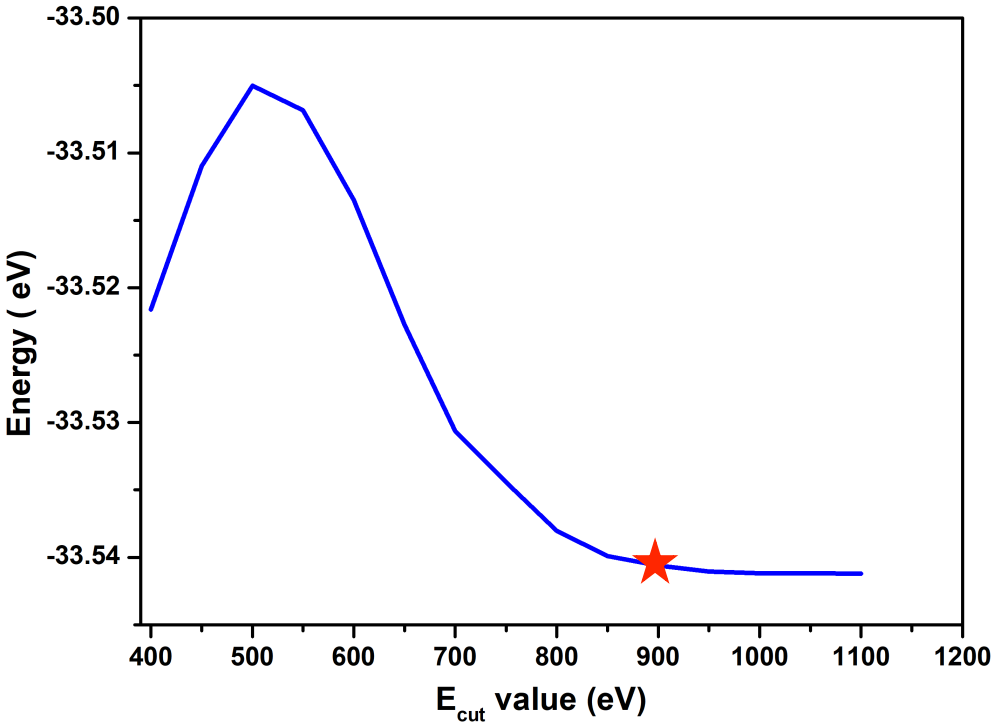

Figure S1: The energy vs cut-off value plot for E_{cut} optimization.

S2: For the thermodynamic feasibility of N doped T-graphene, N doping energy of N doped T-graphene has been computed using the formula:

N doping energy = Energy of N doped T-graphene + Energy of C atoms – Energy of T-graphene – Energy of N atoms

The N doping energy is obtained as -13.154 eV and it validates the effective doping of N in the T-graphene lattice.

S3: T-graphene has also been explored for anode material in alkali ion batteries. The comparison of the results of T-graphene and N doped T-graphene are included in the table below:

	Adsorption Energy (eV)	Diffusion barrier (eV)	Storage Capacity ($mAhg^{-1}$)
T-graphene [1]	-1.26	0.35	2232
N doped T-graphene	-0.21	0.59	754/2140

For the calculation of storage capacity, the formula being used is:

$$C = \frac{enF}{M_f}$$

where *e* is electronic charge, *n* is the number of atoms adsorbed, *F* is Faraday's constant and M_f is the mass of the formula unit.

While calculating the theoretical capacity of T-graphene, the authors from Ref. [1] have taken the mass of formula unit (M_f) corresponding to the stoichiometry Na_6C_6 as mass of C_6. Thus, the value of theoretical capacity is reported as 2232 $mAhg^{-1}$.

We have calculated the theoretical capacity by considering the mass of formula unit as the mass of Na_4C_3N. Therefore, we got the capacity as 754 $mAhg^{-1}$.

If we compute the capacity taking the mass of the formula unit as the mass of C_3N, then our capacity is 2140 $mAhg^{-1}$ which is similar to that calculated for T-graphene.

Therefore, the difference in the value of capacities while comparing them is due to the difference in the stoichiometry considered for the formula unit.

[1] J. Hu, Y. Liu, N. Liu, J. Li and C. Ouyang*, Phys. Chem. Chem. Phys.*, 2020, **22**, 3281-3289.