Supplementary Information

Two-dimensional graphene+ as an anode material for calcium-ion batteries with ultra-high capacity: a first-principles study

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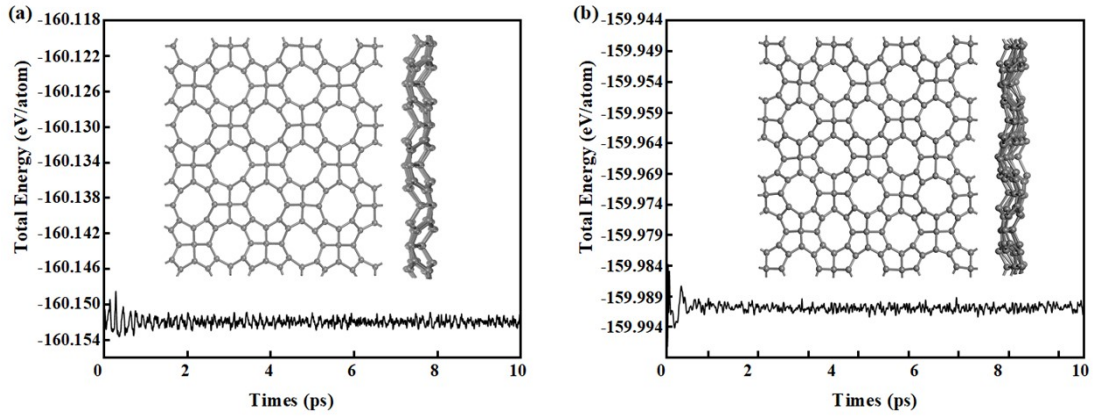

Fig. S1 Variation in total energy at 400 (a) and 800 K (b) using AIMD simulation for graphene+.

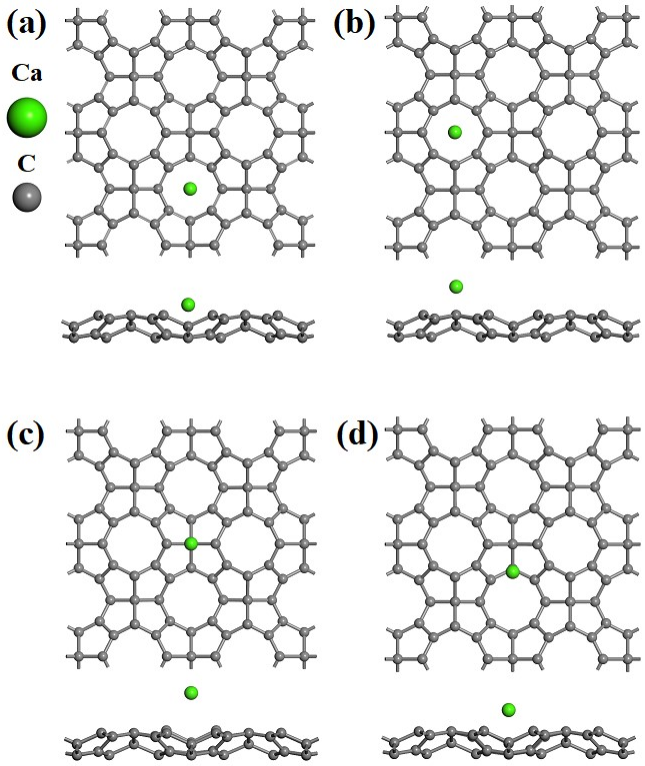

Fig. S2 (a)-(d) Four stable adsorption sites of Ca on graphene+.

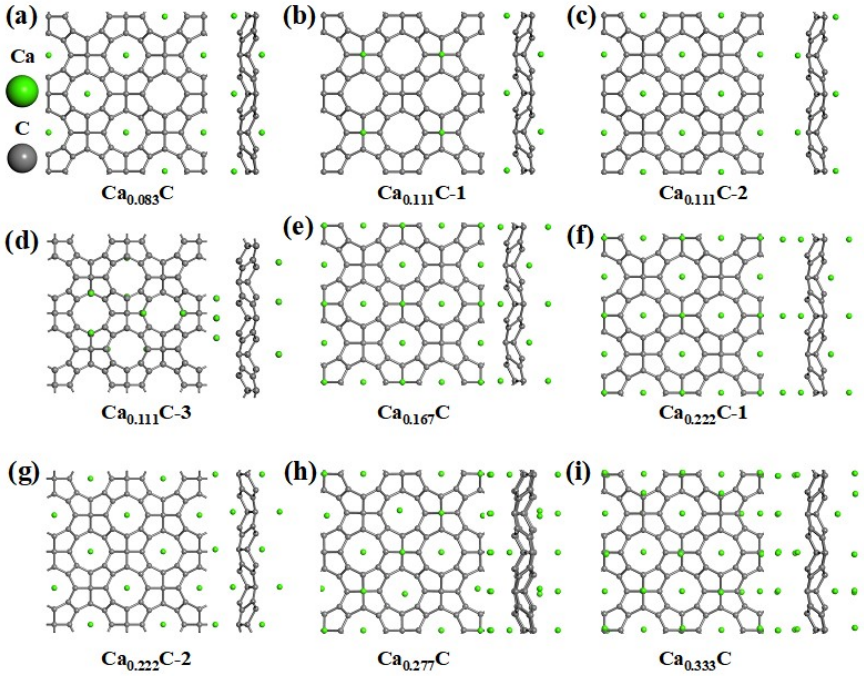

Fig. S3 Meta-stable configurations of graphene+ with different Ca concentrations.

Table S1 The possible adsorption and final (after relax) adsorption sites.

Possible adsorption site	Final adsorption site
$H_1/T_5/B_1$	H_1
H_2	H_2
$T_1/T_3/T_4$	T_1
$T_2/H_3/T_4/B_2/B_3/B_5$	T_2

Table S2 Description of graphene+ phases with different Ca concentrations. The structures marked with an asterisk (*) represent stable phases located at the minima of the convex curve.

Stoichiometry	Distance to the convex hull (eV per formula unit)
C*	0.0
$Ca_{0.027}C$*	0.0
$Ca_{0.055}C$*	0.0
$Ca_{0.083}C$	0.03
$Ca_{0.083}C$*	0.0
$Ca_{0.111}C$-1	0.31
$Ca_{0.111}C$-2	0.44
$Ca_{0.111}C$-3	0.55
$Ca_{0.111}C$*	0.0
$Ca_{0.167}C$	0.02
$Ca_{0.222}C$-1	0.57
$Ca_{0.222}C$-2	0.65
$Ca_{0.222}C$*	0.0
$Ca_{0.277}C$	0.09
$Ca_{0.333}C$	0.20
$Ca_{0.333}C$*	0.0