Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First principles studies of two dimensional C-Silicyne nanosheet as a promising anode material for rechargeable Li-ion batteries

Nidhi Duhan[1], and T. J. Dhilip Kumar[1*]
[1]*Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar 140001, India*

*Email: dhilip@iitrpr.ac.in

(1) Coordinates of C-Silicyne unit cell:

C	1.5241676542	3.8814647503	5.0000000000
C	0.0000002805	6.5214006810	5.0000000000
C	1.5241676542	3.8814650361	5.0000000000
C	2.5993631723	3.2607008618	5.0000000000
C	4.1235306862	0.6207649312	5.0000000000
C	5.6476986168	3.2607002977	5.0000000000
Si	4.1235309626	2.3807219683	5.0000000000
Si	0.0000000000	4.7614433654	5.0000000000

(2) Systematic loading of Li-atoms over C-Silicyne monolayer:

Li atoms are added step by step, 2 atoms at a time. Firstly, all the 8 sites above the monolayer were loaded with Li atom, making the layer1. Then, Li atoms are added below the monolayer over the site E (which is the most favourable site). Only 6 of them were able to take up the Li atoms (making the layer2), further the monolayer started to collapse. But adsorption energies are still high, so next Li atoms were added to site B, which is the next preferred site. It could take up 2 more Li atoms. After that the monolayer started to distort, a total of 16 Li atoms could be loaded. (If we add 2nd layer over site B instead of site E, then also only 16 Li atoms could be loaded in total, as after 16 atoms, the formation energy became positive.) Following Figure shows systematic loading of Li atoms over C-Silicyne monolayer:

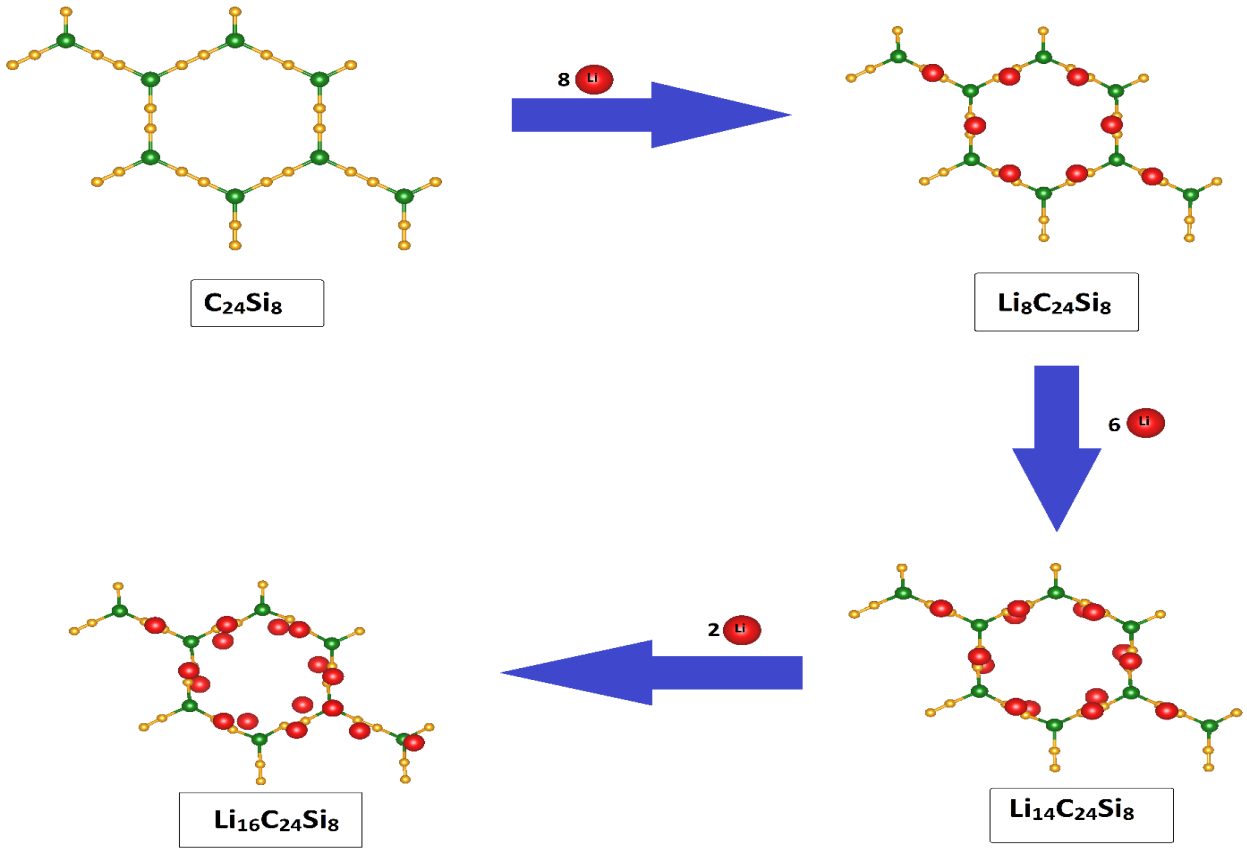

Figure S1 Systematic Li adsorption over the C-Silicyne monolayer.

(3) Formation Energy:

Formation energy is calculated using the equation:

$$E_f = (E_{CS\text{-}Li} - E_{CS} - nE_{Li})/n$$

Where,
$E_{CS\text{-}Li}$ = Energy of Li adsorbed C-Silicyne monolayer,
E_{CS} = Energy of C-Silicyne monolayer,
E_{Li} = Energy of Li in metallic bulk,
n = Number of Li atoms adsorbed.

(4) Coverage ratio of Li atom:

Supercell =$C_{24}Si_8$ Formula unit = C_3Si

Li loading :

Table S1 Coverage ratio calculation.

System	Formula unit	Coverage ratio(r)
$Li_2C_{24}Si_8$	$Li_{0.25}C_3Si$	0.25
$Li_4C_{24}Si_8$	$Li_{0.50}C_3Si$	0.50
$Li_6C_{24}Si_8$	$Li_{0.75}C_3Si$	0.75
$Li_8C_{24}Si_8$	Li_1C_3Si	1.00
$Li_{10}C_{24}Si_8$	$Li_{1.25}C_3Si$	1.25
$Li_{12}C_{24}Si_8$	$Li_{1.50}C_3Si$	1.50
$Li_{14}C_{24}Si_8$	$Li_{1.75}C_3Si$	1.75
$Li_{16}C_{24}Si_8$	Li_2C_3Si	2.00

(5) Diffusion path B:

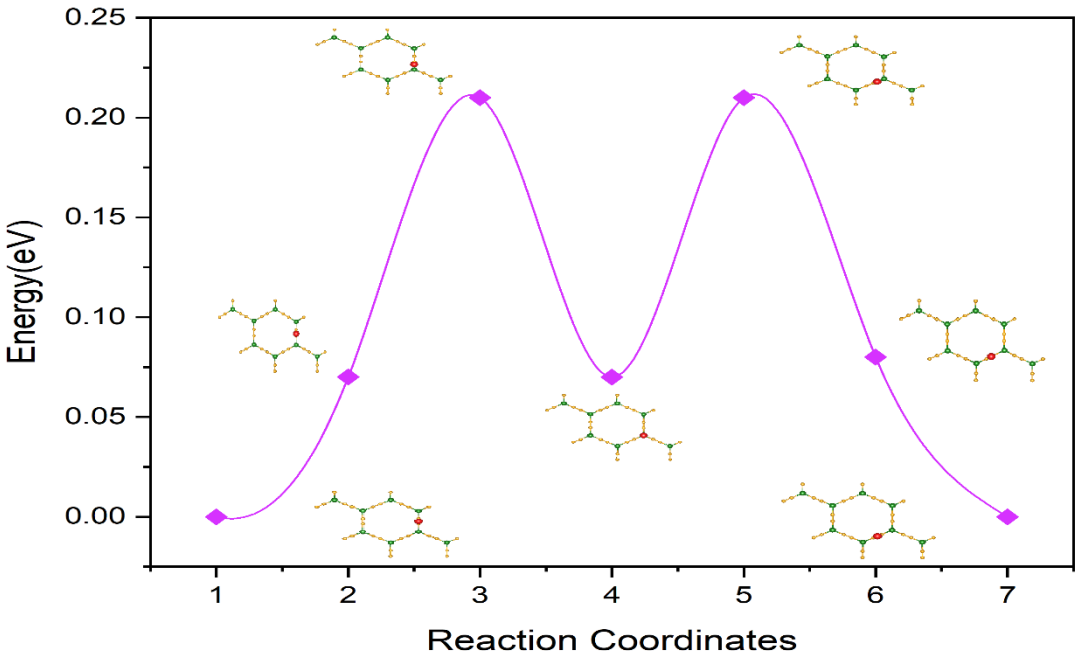

Fig S2 Relative energy profile of migration pathway B with structures.

(6) Side view of C-Silicyne nanosheet representing adsorption distance h.

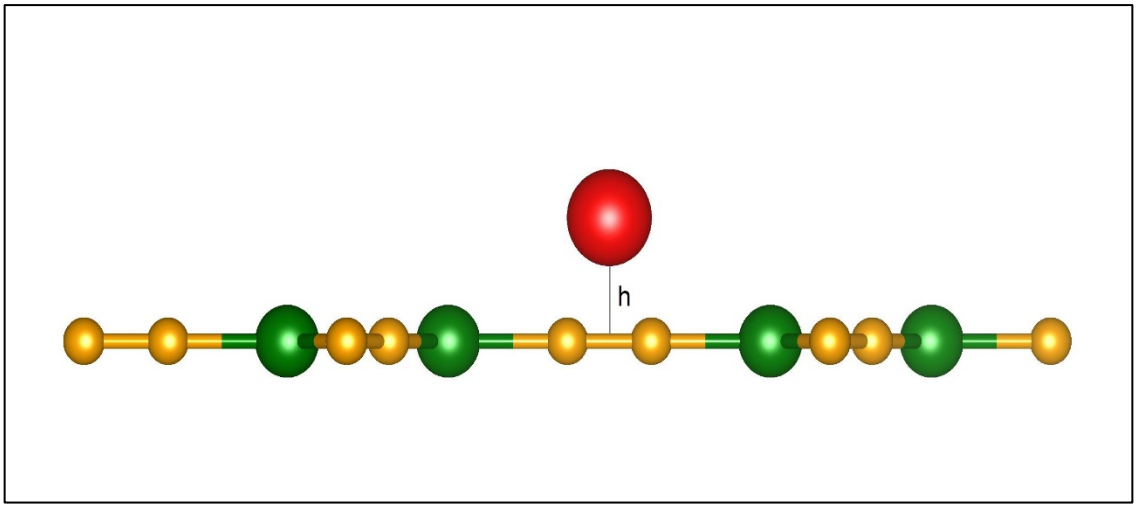

Fig S3 Side view of C-Silicyne nanosheet depicting the distance (h) of adatom from the nanosheet.

(7) Relative change in the area of xy-plane of the nanosheet.

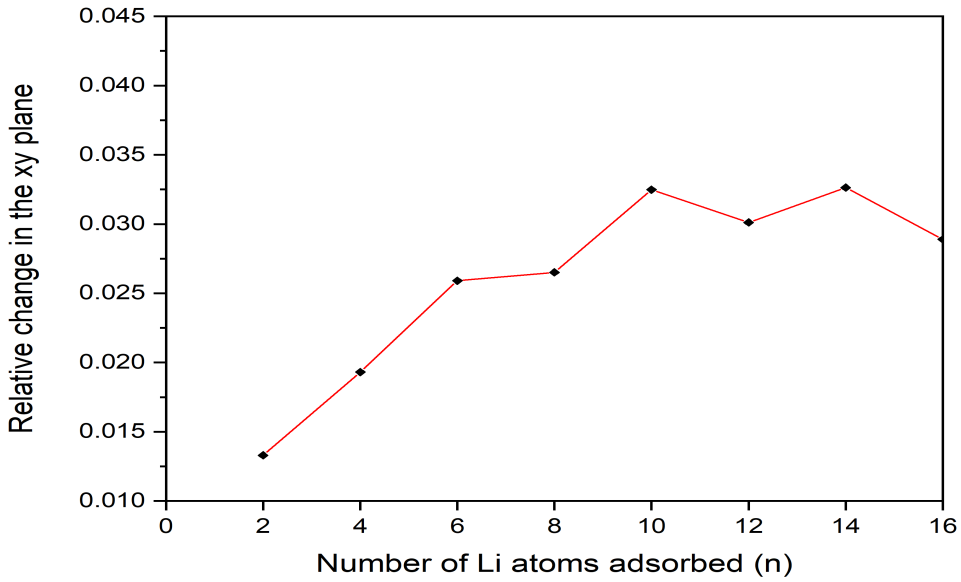

Fig S4 Relative change in area of xy plane of C-Silicyne as a function of Li loading.