Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting Information for

Prediction of Two Dimensional CP_3 as a Promising Electrode Material with a Record-High Capacity for Na Ions

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Contents of Supporting Information

1. The cleavage energy of CP_3 monolayer (Figure S1).
2. The optimized structures of CP_3 monolayer adsorption Li/Na (Figure S2).
3. Mechanical parameters for the CP_3 monolayer before and after adsorption Li/Na (Table S1).

1. Cleavage Energy: Cleavage energy was calculated by using five-layers system as shown in the following figure, and the value was calculated by the following formula:

$$E_{cleavage} = (E_{5L+d} - E_{5L})/S$$

Where $E_{cleavage}$, E_{5L+d}, E_{5L}, and S represent the cleavage energy, the total energy of 5L slab with and without displacement, and the total area of the unit cell, respectively. From the Figure S1, we find that the cleavage energy of CP_3 is 0.65 J/m^2 and agrees with the previous work (0.57 J/m^2) [*Phys. Rev. B. 2020, 101, 195305*]. And this low value suggests that CP_3 monolayer could be cleavable from its bulk structure.

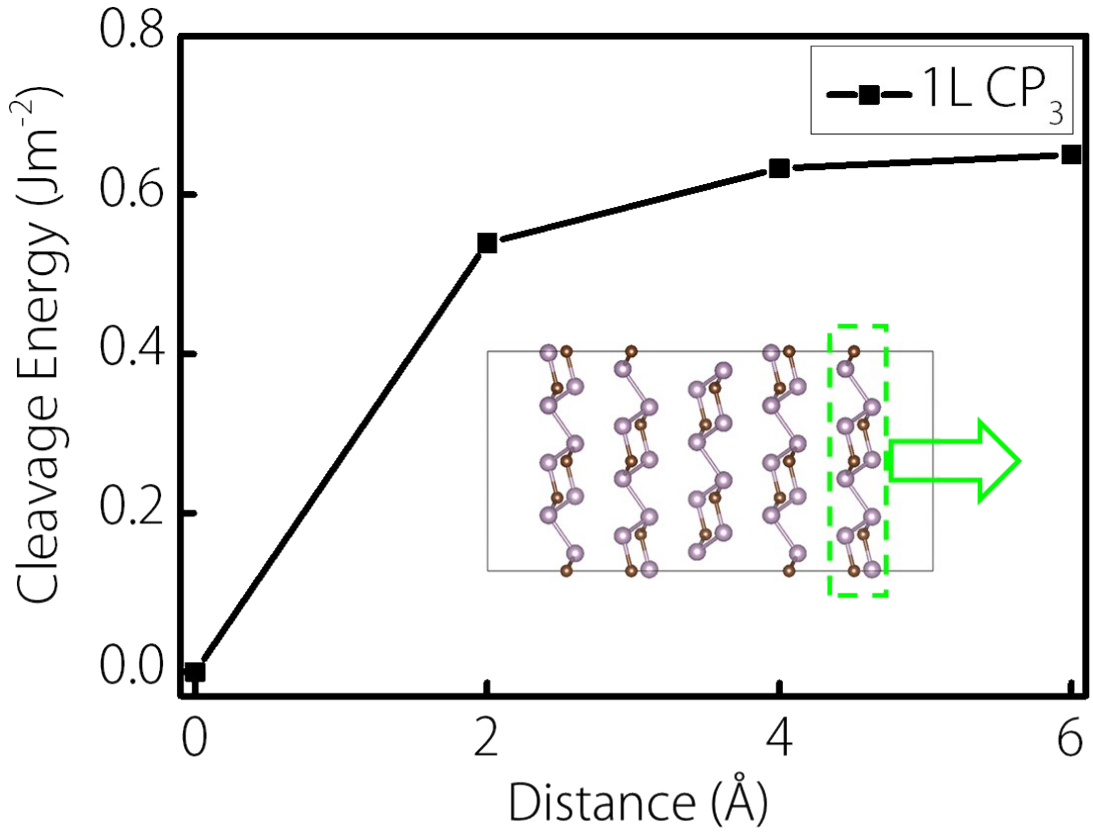

Figure S1 Cleavage energy of CP_3 is as a function of the separation distance between 1L and the remainder of the 5L-slab. The distance changes from 0 to 6 Å, and the distance zero means the equilibrium distance of the bulk structure. The 5L-slab is shown in map.

2.

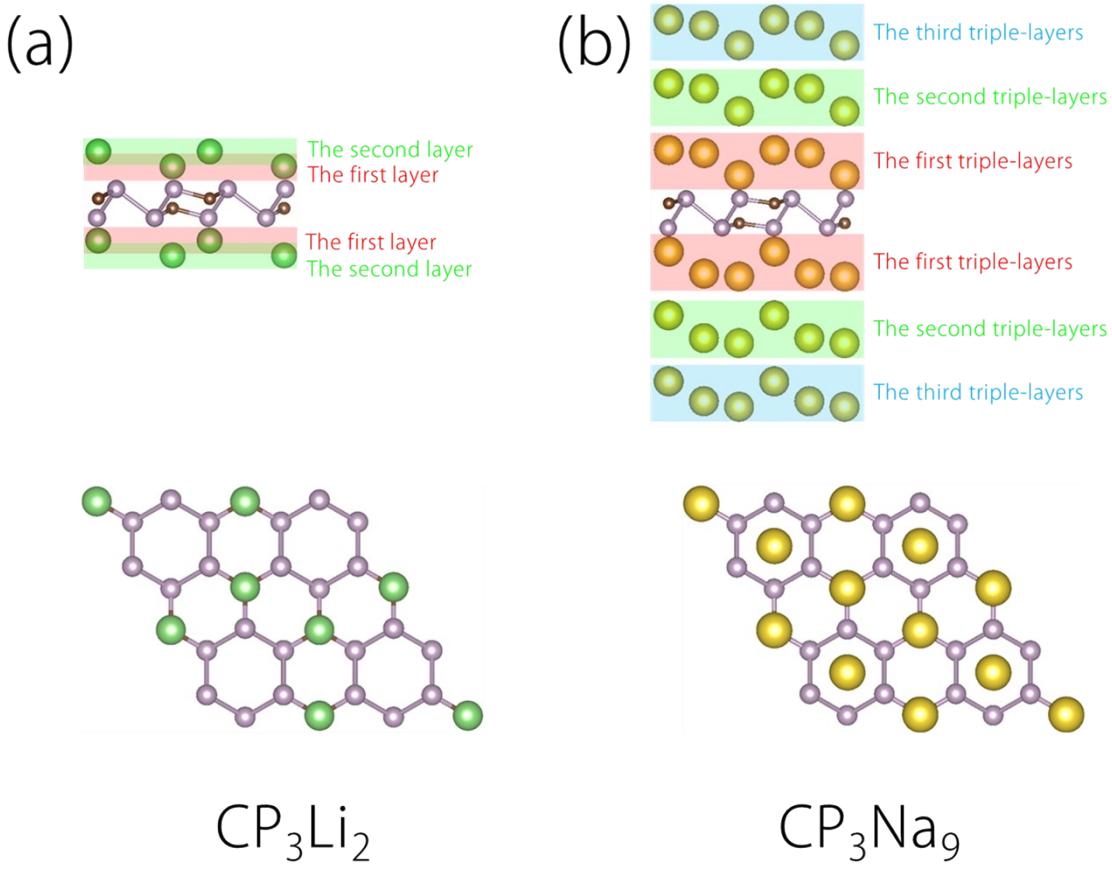

Figure S2 (a) The optimized structure of CP_3Li_2 on the top and side views. (b) The optimized structure of CP_3Na_9 on the top and side views. And the number of layers is marked in their top views.

3. The elastic constants of CP_3 monolayer are $C_{11} = C_{22} = 83.7$ N/m, $C_{12} = 19.1$ N/m, and $C_{44} = 32.5$ N/m. After adsorption Li/Na atoms, we find the elastic constants of CP_3 monolayer have not changed much. And these values all satisfy the Born criteria ($C_{44} > 0; C_{11}C_{22} - C_{12}^2 > 0$), which indicates the CP_3 monolayer before and after adsorption Li/Na are mechanically stable. Besides, the Young modulus could be calculated by $E = (C_{11}^2 - C_{12}^2)/C_{11}$ and the Poisson ratio is $\nu = C_{12}/C_{11}$. The results are shown in the Table S1.

Table S1 Mechanical parameters for the CP_3 monolayer before and after adsorption Li/Na

	C_{11} (N/m)	C_{22} (N/m)	C_{44} (N/m)	C_{12} (N/m)	E (N/m)	ν
before	83.7	83.7	32.5	19.1	79.3	0.23
After Li	81.9	81.9	33.4	15.1	79.1	0.18
After Na	78.2	78.2	30.1	17.9	74.1	0.23