

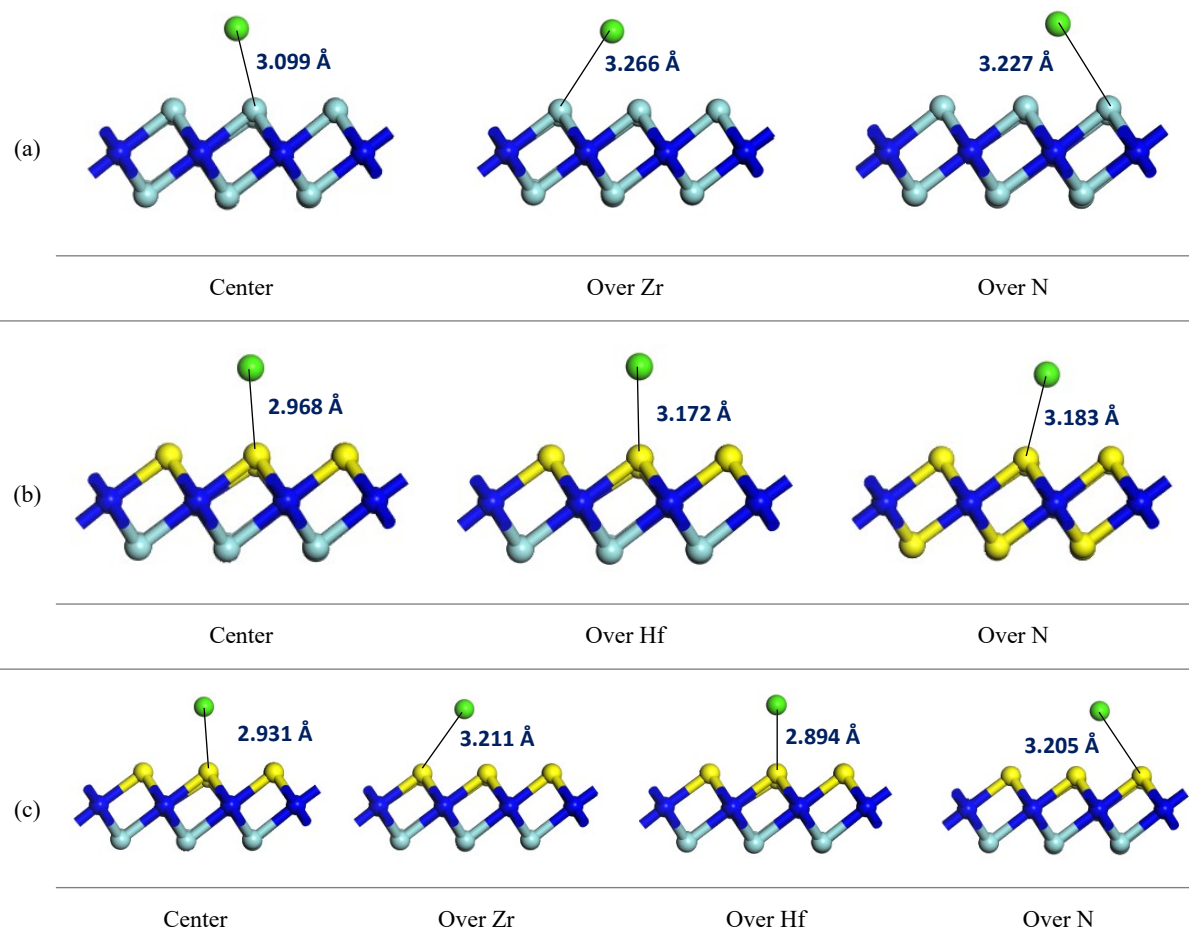
## Supplementary Information

### Recent Advances in Zr and Hf-based MXenes and their Hetero-structure as Novel Anode Materials for Ca-ion batteries: A Theoretical Insight from DFT Approach

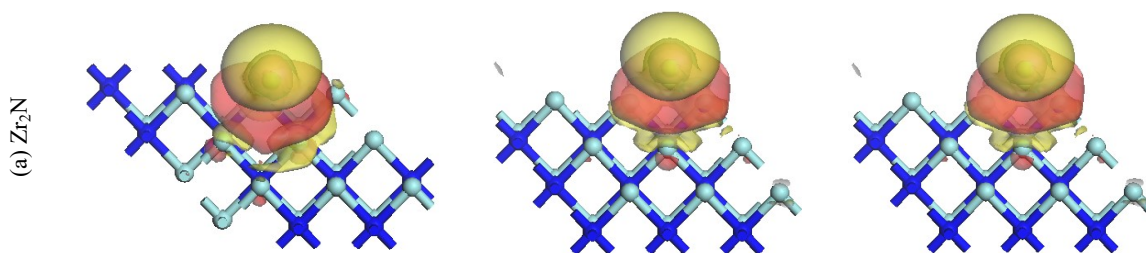
Tanvir Ahmed <sup>a</sup>, Afiya Akter Piya <sup>a</sup> and Siraj Ud Daula Shamim <sup>a\*</sup>

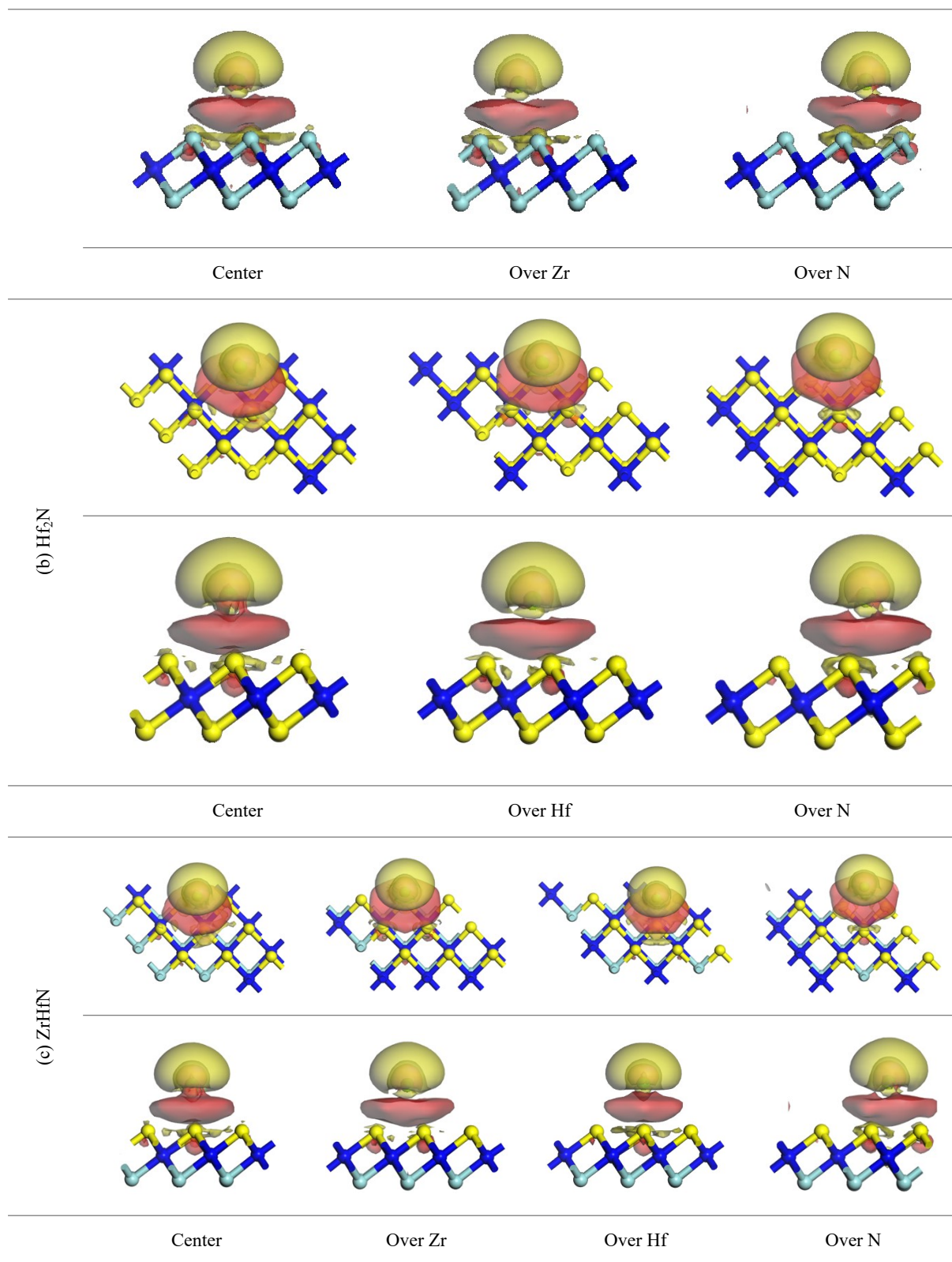
Department of Physics, Mawlana Bhashani Science and Technology University, Tangail, Bangladesh.

\*Corresponding Author: Siraj Ud Daula Shamim ([sdshamim@mbstu.ac.bd](mailto:sdshamim@mbstu.ac.bd))

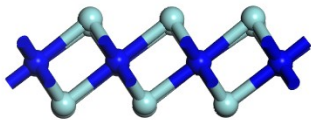
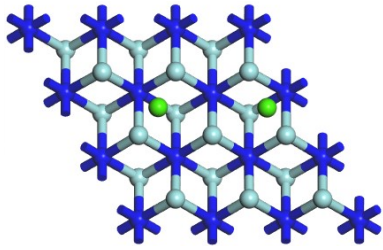


**Figure S1:** Minimum interaction distance between Ca adatom and MXenes.

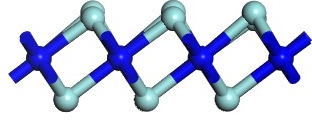
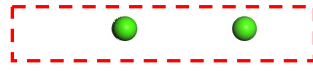
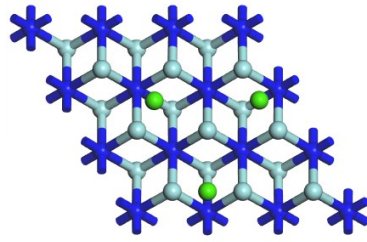




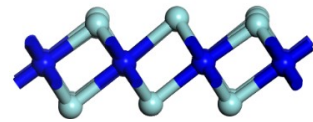
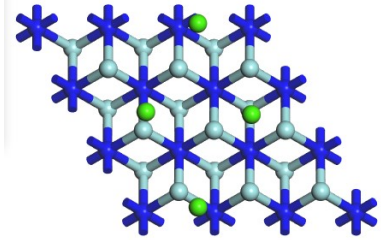
**Figure S2:** The CDD map of a single Ca loaded (a) Zr<sub>2</sub>N, (b) Hf<sub>2</sub>N and (c) ZrHfN. Where isosurface was set at  $0.01 e/\text{\AA}^{-3}$ .



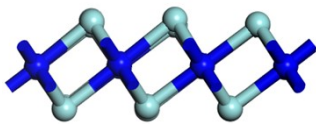
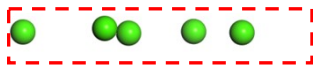
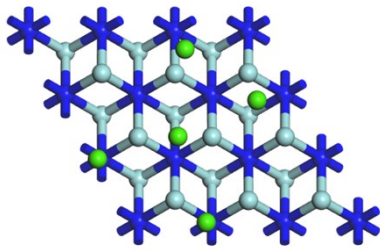
(a) 2 Ca



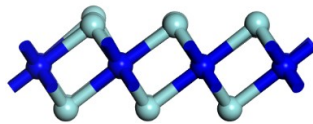
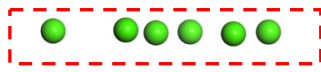
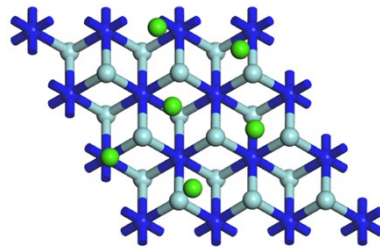
(b) 3 Ca



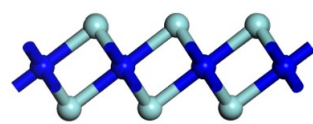
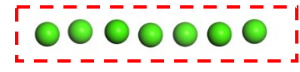
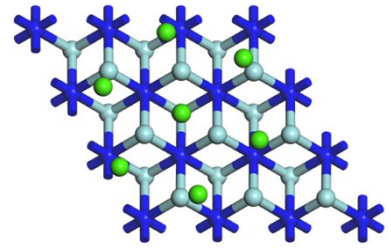
(c) 4 Ca



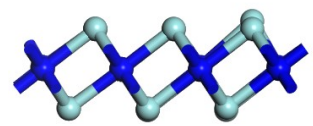
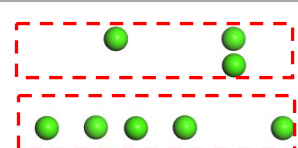
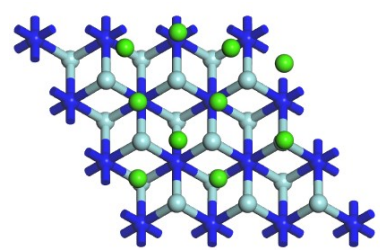
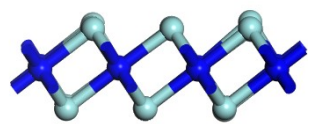
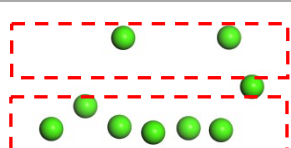
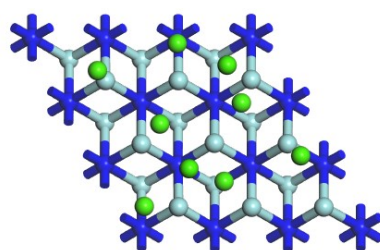
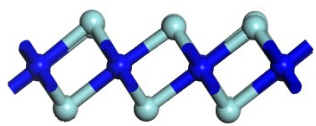
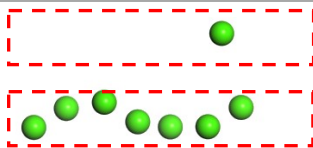
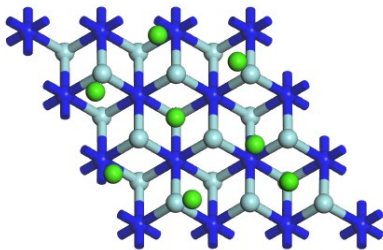
(d) 5 Ca



(e) 6 Ca

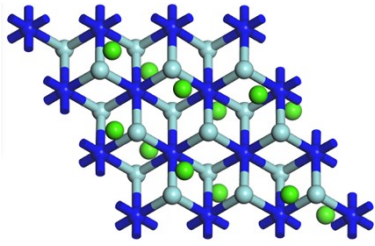


(f) 7 Ca

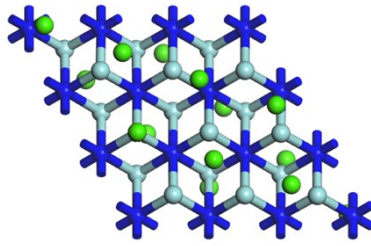




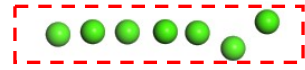
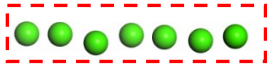
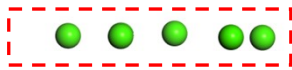
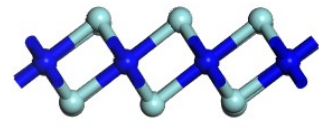
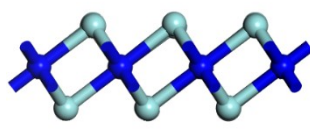
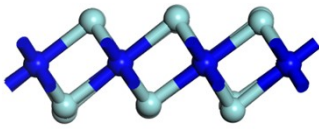
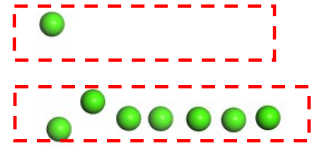
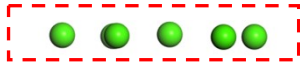
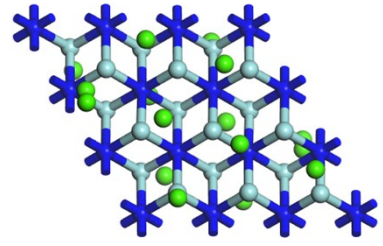
(g) 8 Ca



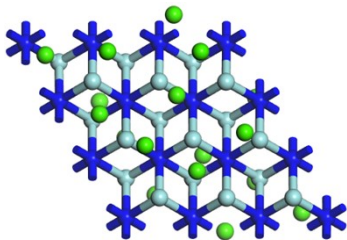
(h) 9 Ca



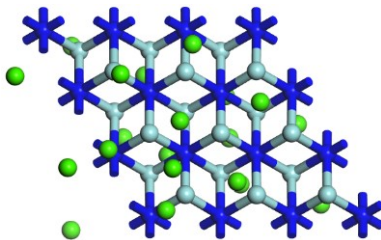
(i) 10 Ca



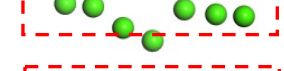
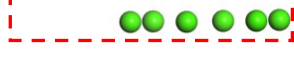
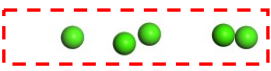
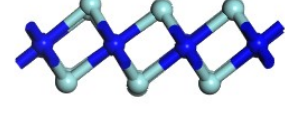
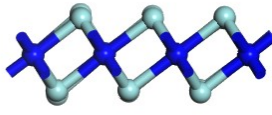
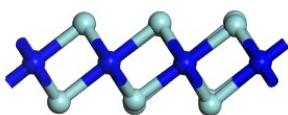
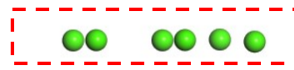
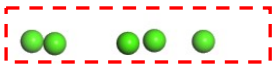
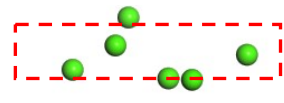
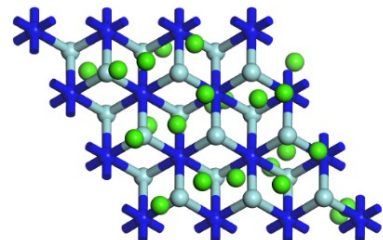
(j) 12 Ca

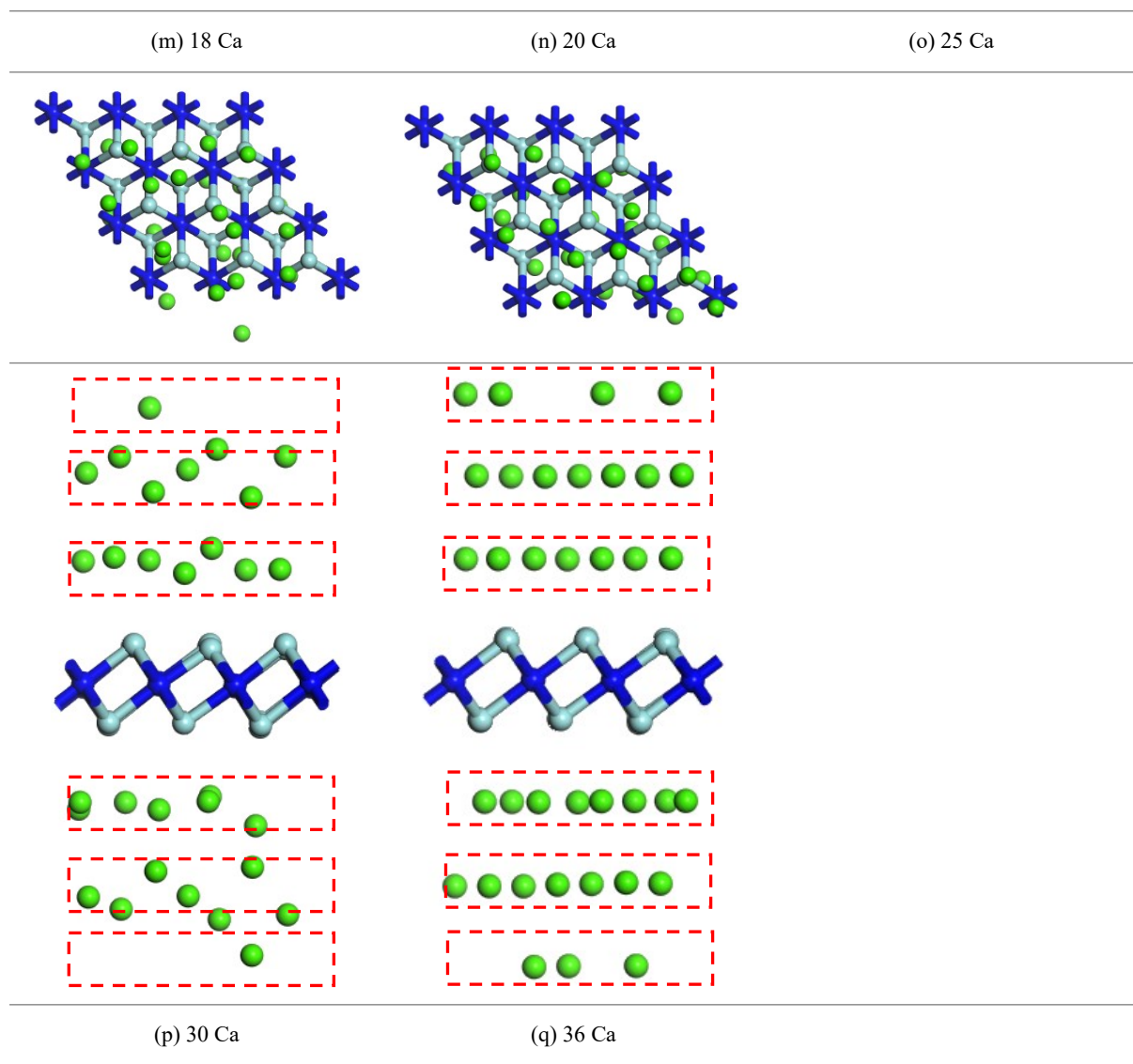


(k) 14 Ca

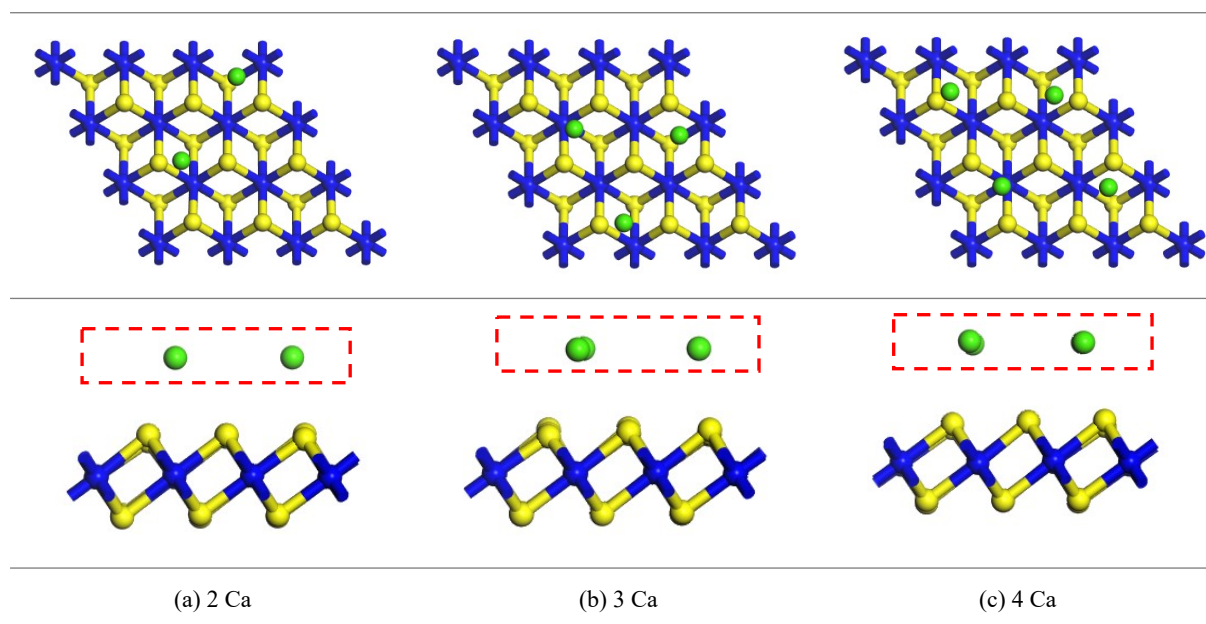


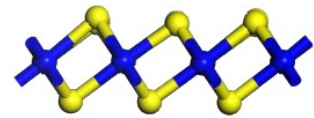
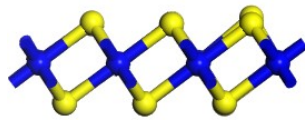
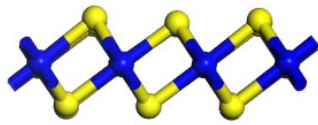
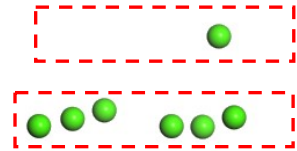
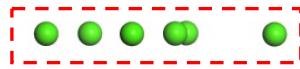
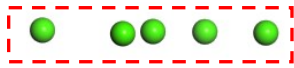
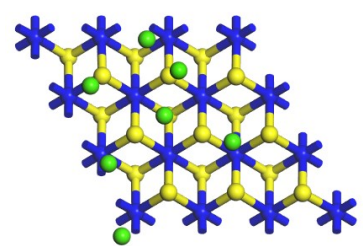
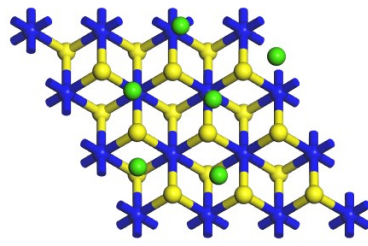
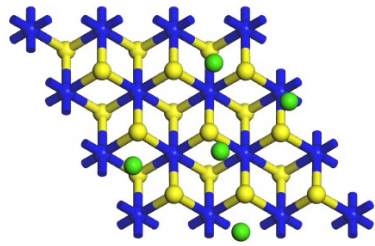
(l) 16 Ca





**Figure S3:** Top and side view of the Ca adsorption on  $Zr_2N$ .

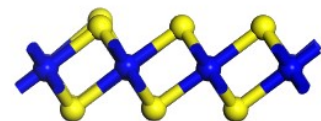
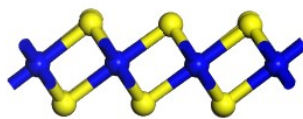
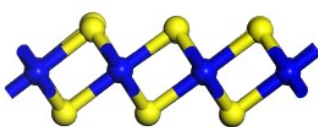
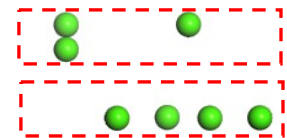
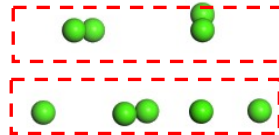
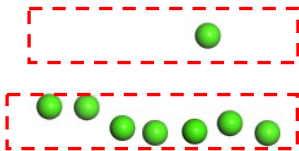
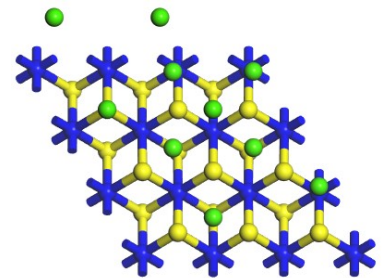
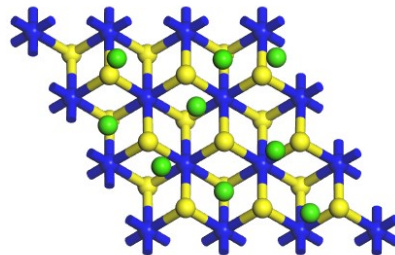
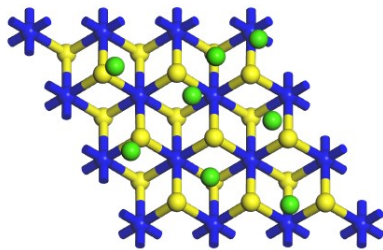




(d) 5 Ca

(e) 6 Ca

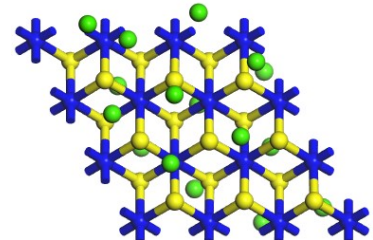
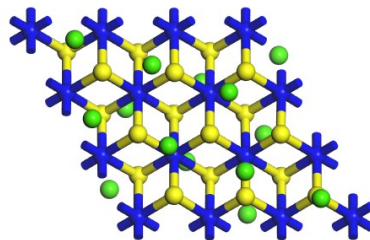
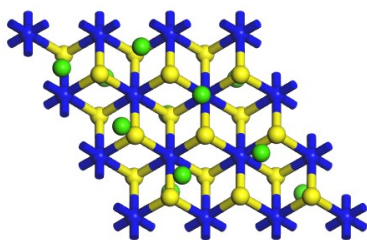
(f) 7 Ca



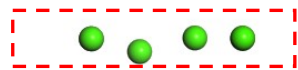
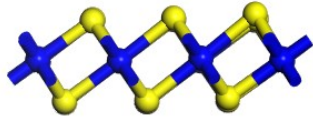
(g) 8 Ca

(h) 9 Ca

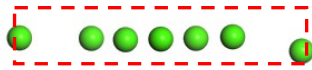
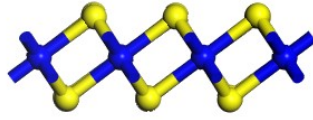
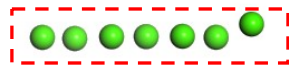
(i) 10 Ca



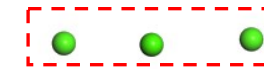
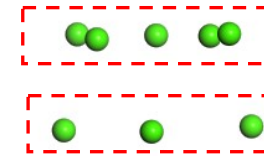
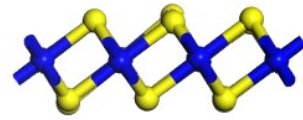
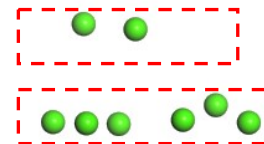




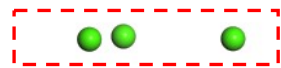
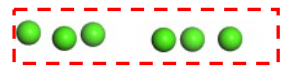
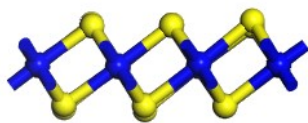
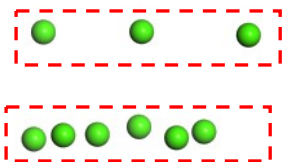
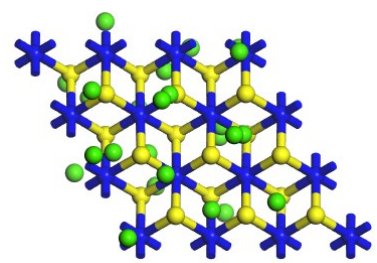
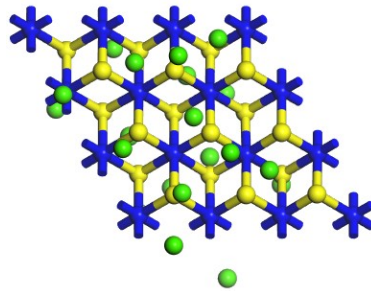
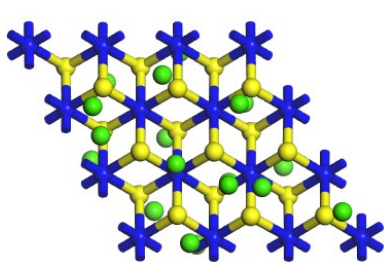
(j) 12 Ca



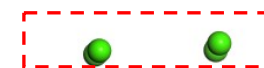
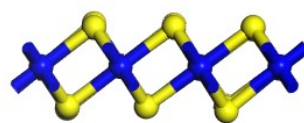
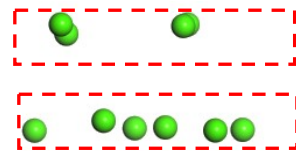
(k) 14 Ca



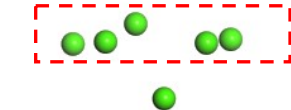
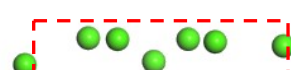
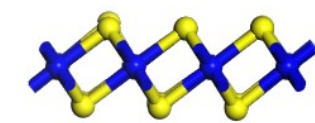
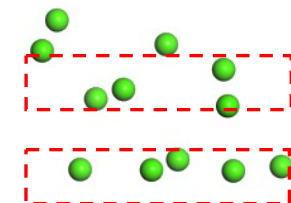
(l) 16 Ca



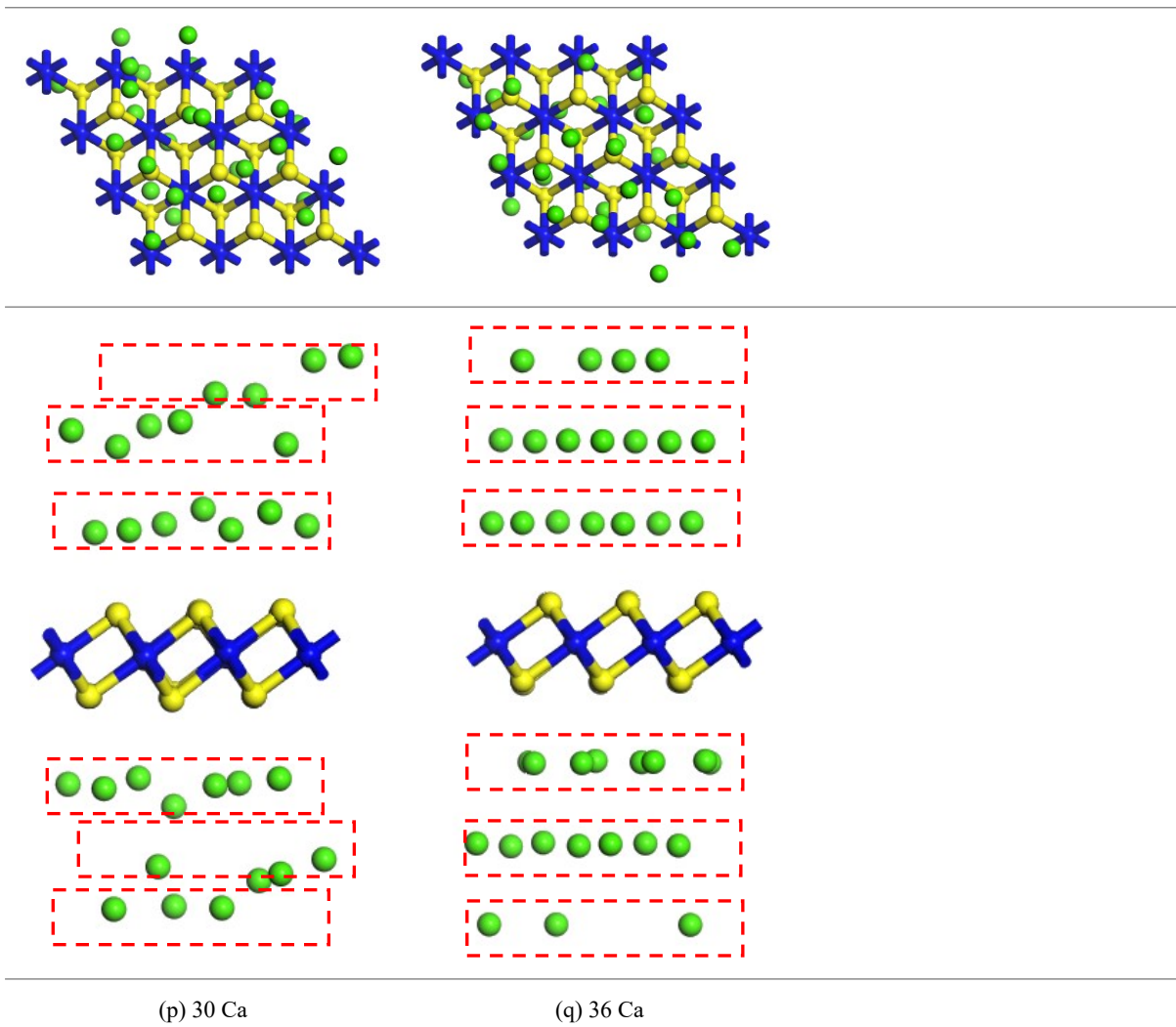
(m) 18 Ca



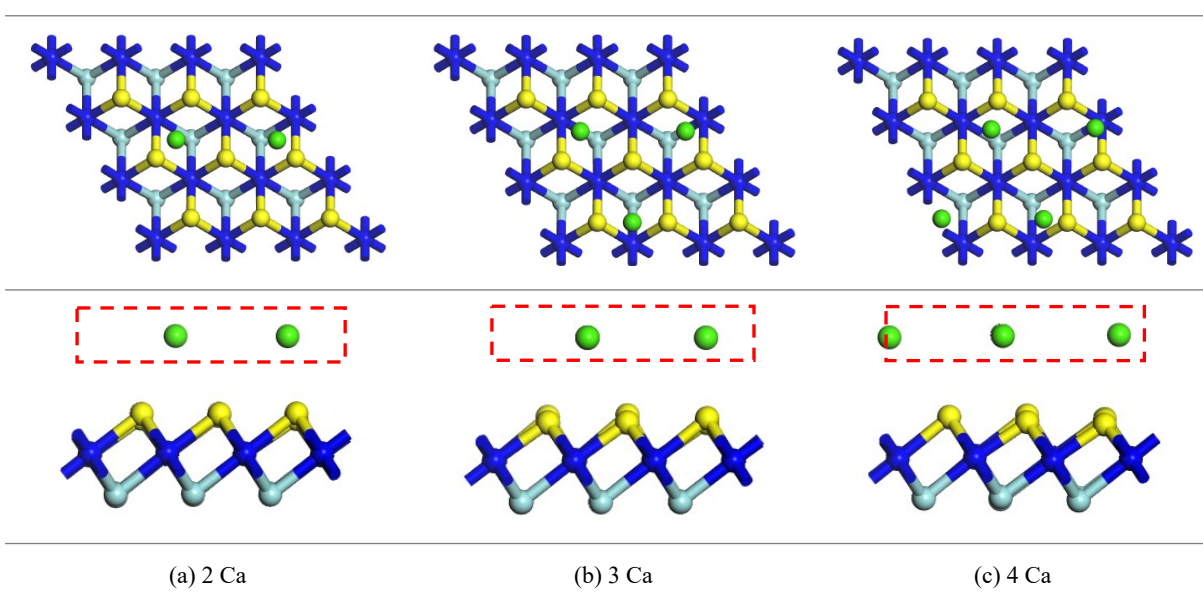
(n) 20 Ca



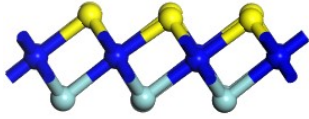
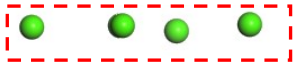
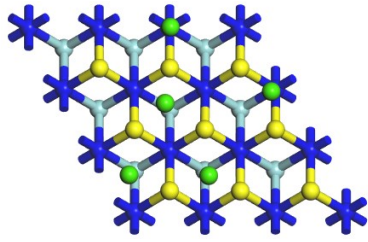
(o) 25 Ca



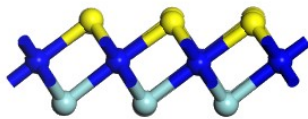
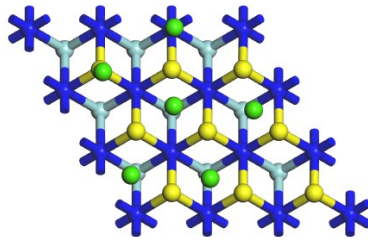
**Figure S4:** Top and side view of the Ca adsorption on Hf<sub>2</sub>N.



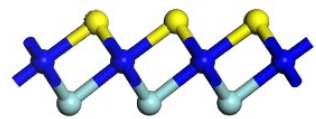
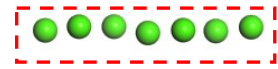
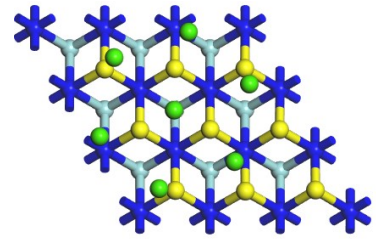




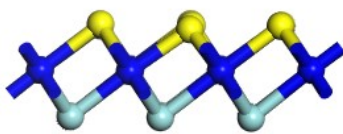
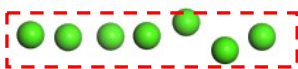
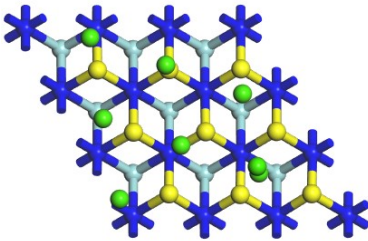
(d) 5 Ca



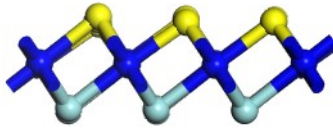
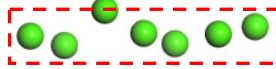
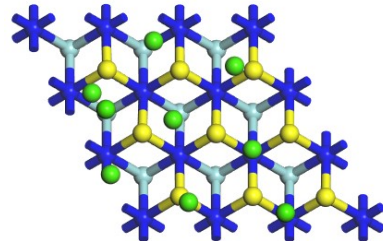
(e) 6 Ca



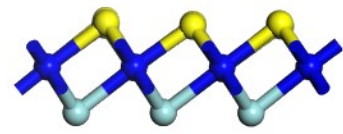
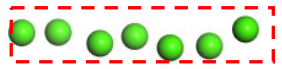
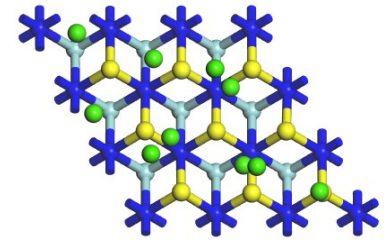
(f) 7 Ca



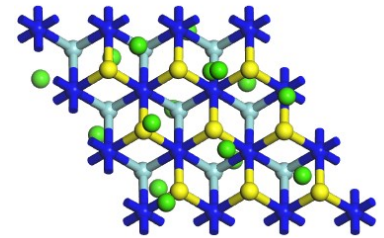
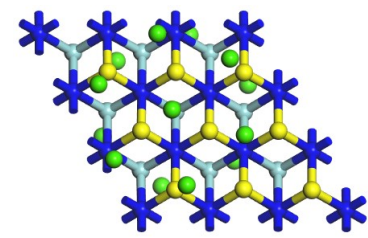
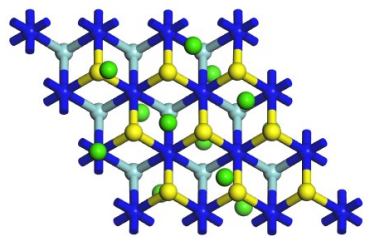
(g) 8 Ca

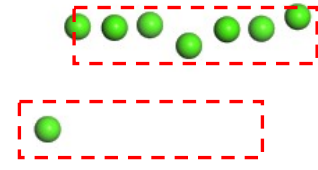
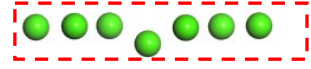
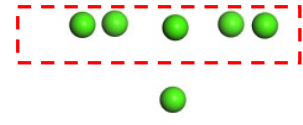
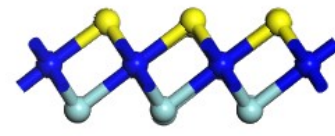
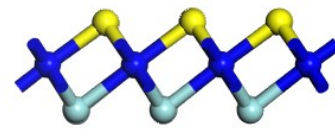
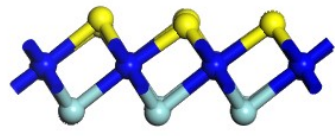
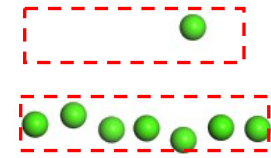
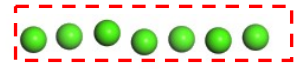
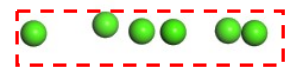


(h) 9 Ca



(i) 10 Ca

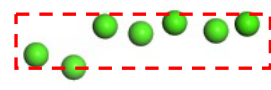
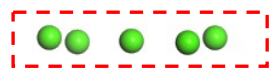
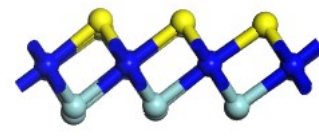
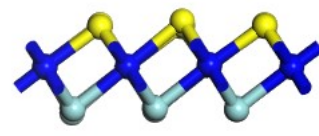
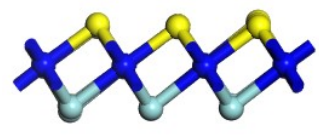
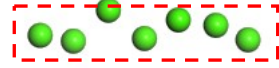
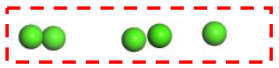
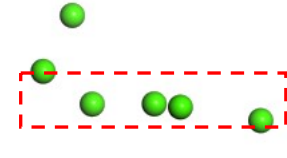
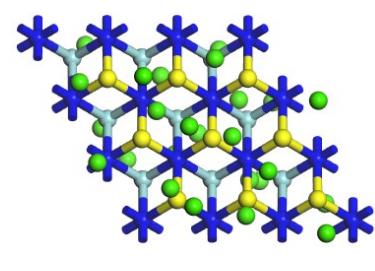
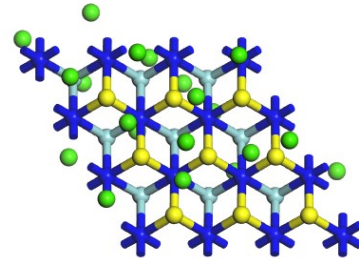
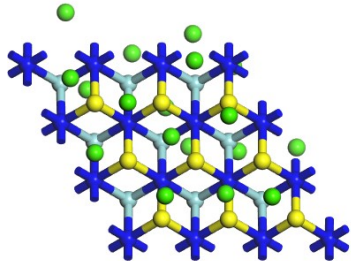




(j) 12 Ca

(k) 14 Ca

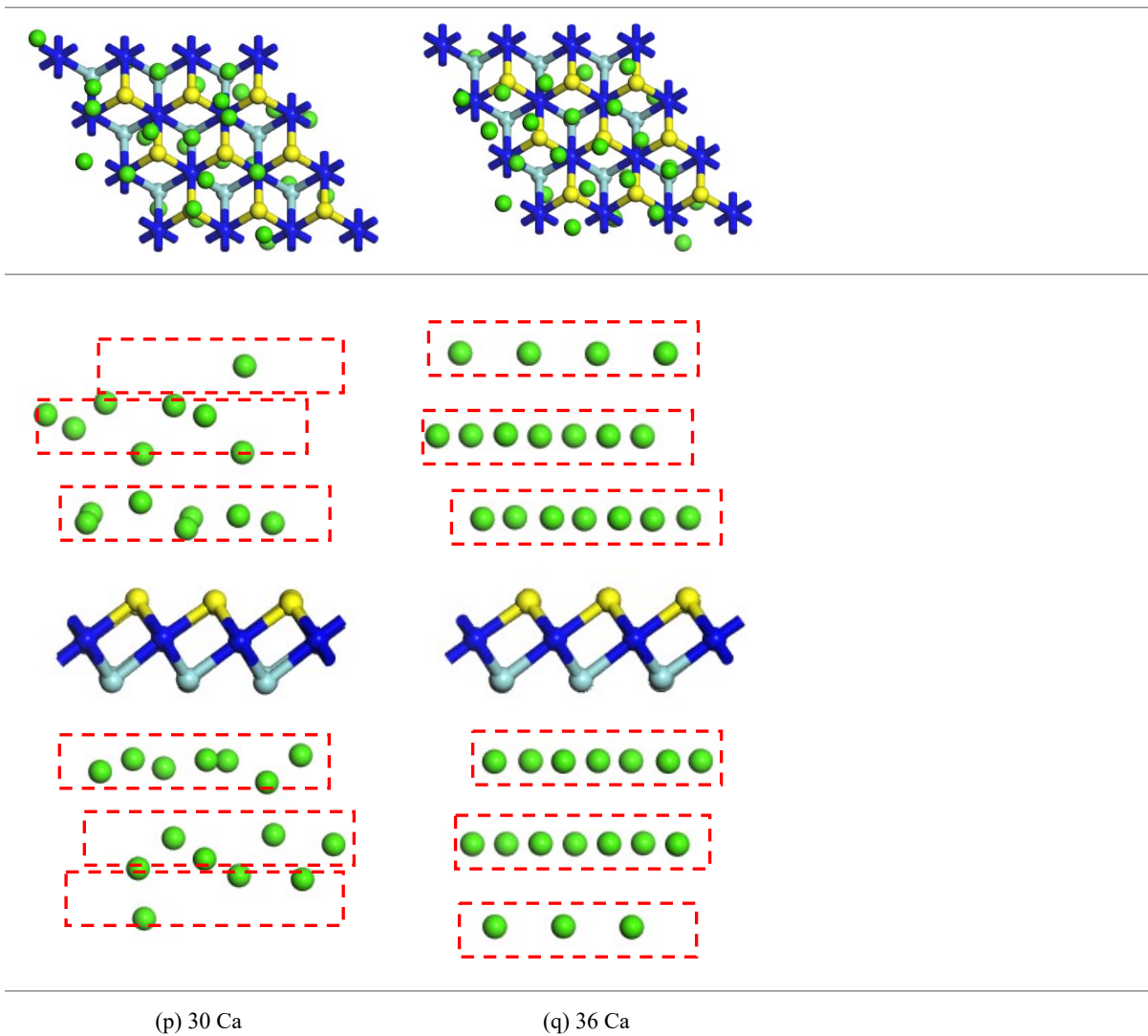
(l) 16 Ca



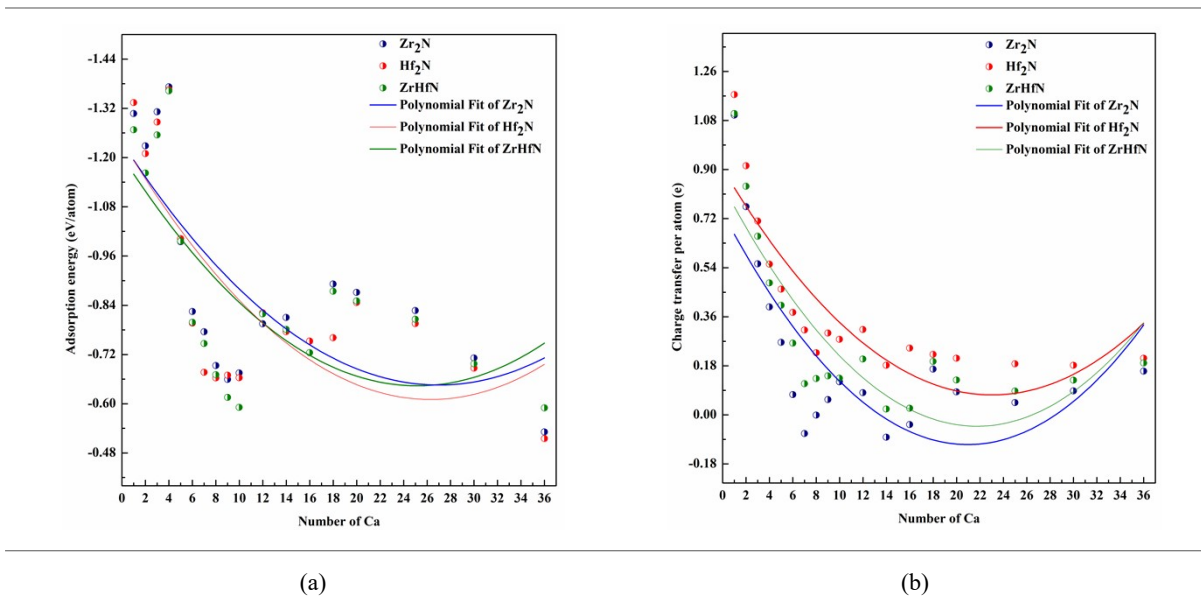
(m) 18 Ca

(n) 20 Ca

(o) 25 Ca



**Figure S5:** Top and side view of the Ca adsorption on ZrHfN.



**Figure S6:** The graphical representation of (a) adsorption energy and (b) charge transfer with increasing the number of Ca on  $Zr_2N$ ,  $Hf_2N$  and  $ZrHfN$ .