# Supporting Information

# Graphene-like Carbon–Nitride Monolayer: A Potential Anode Material for Na and K-ion Batteries

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**Figure S1:** Total and projected density of states of $C_3N$ monolayer.
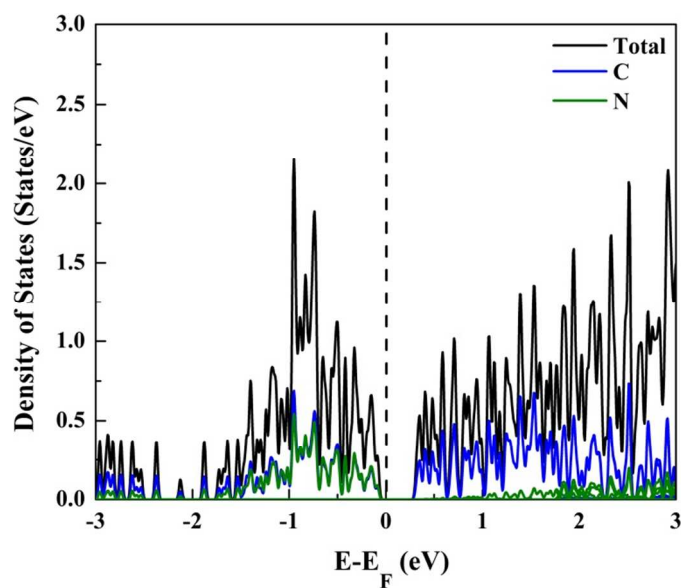
**Figure S2:** Considered adsorption sites for Na and K-ion adsorption on $C_3N$ monolayer surface.
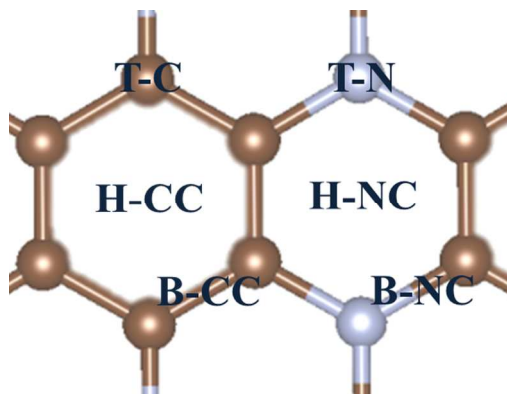
**Table S1:** Calculated adsorption energies and charge transfer values for Na and K adsorption on $C_3N$ surface.

| Sites | Na | | | K | | |
|-------|-----|-----|-----|-----|-----|-----|
| | Total Energy (eV) | Adsorption Energy (eV) | Charge transfer (\|e\|) | Total Energy (eV) | Adsorption Energy (eV) | Charge transfer (\|e\|) |
| H-CC | -635.79459 | -1.806 | 0.63 | -635.96788 | -2.230 | 0.69 |
| H-NC | -635.76505 | -1.777 | 0.62 | -635.92326 | -2.180 | 0.67 |
| T-N | -635.76380 | -1.775 | 0.62 | -635.92862 | -2.191 | 0.67 |

**Figure S3:** Adsorption structures of Na adsorption layer on $C_3N$ surface, (a) first, (b) second, (c) third, (d) fourth, and (e) fifth adsorption layer.
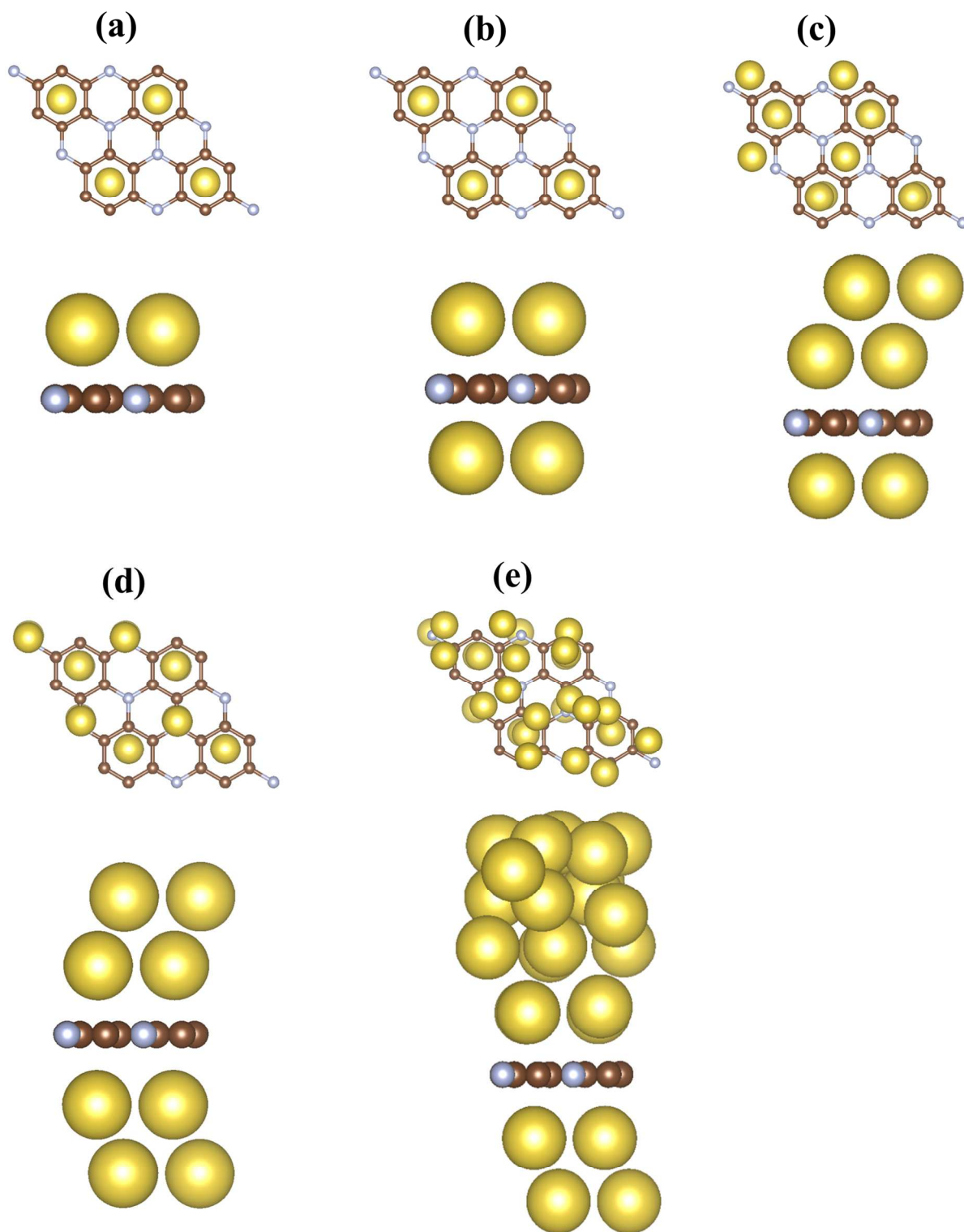
**Figure S4:** Adsorption structures of K adsorption layer on $C_3N$-surface, (a) first, (b) second, (c) third, (d) fourth, and (e) fifth adsorption layer.