Electronic Supplementary Material (ESI)

# Prediction of chemically ordered dual transition metal carbides (MXenes) as high-capacity anode materials for Na-ion batteries

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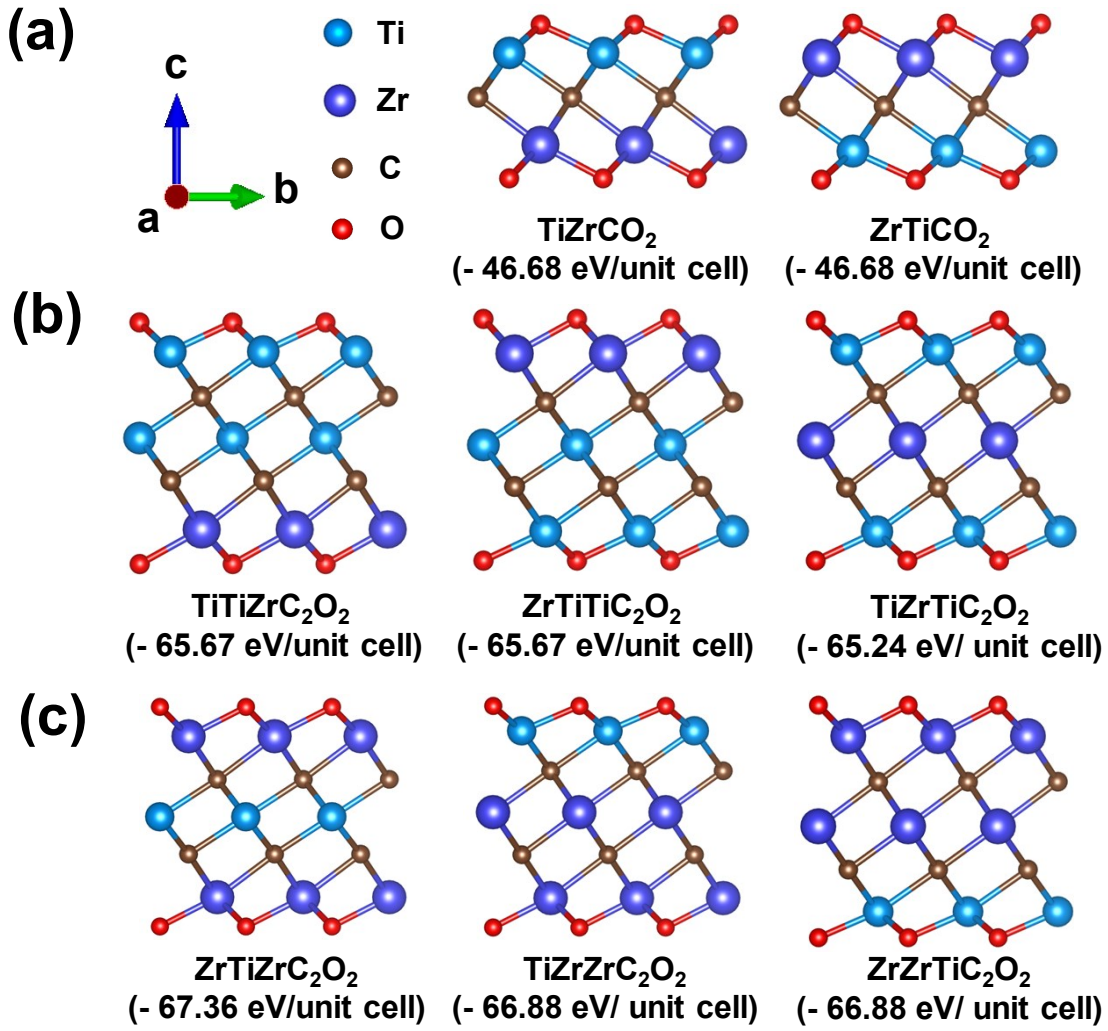


**Figure S1.** Optimized structures of potential configurations of (a) $TiZrCO_2$, (b) $Ti_2ZrC_2O_2$ and (b) Ti $Zr_2C_2O_2$. The calculated total energies of these structures are also given.

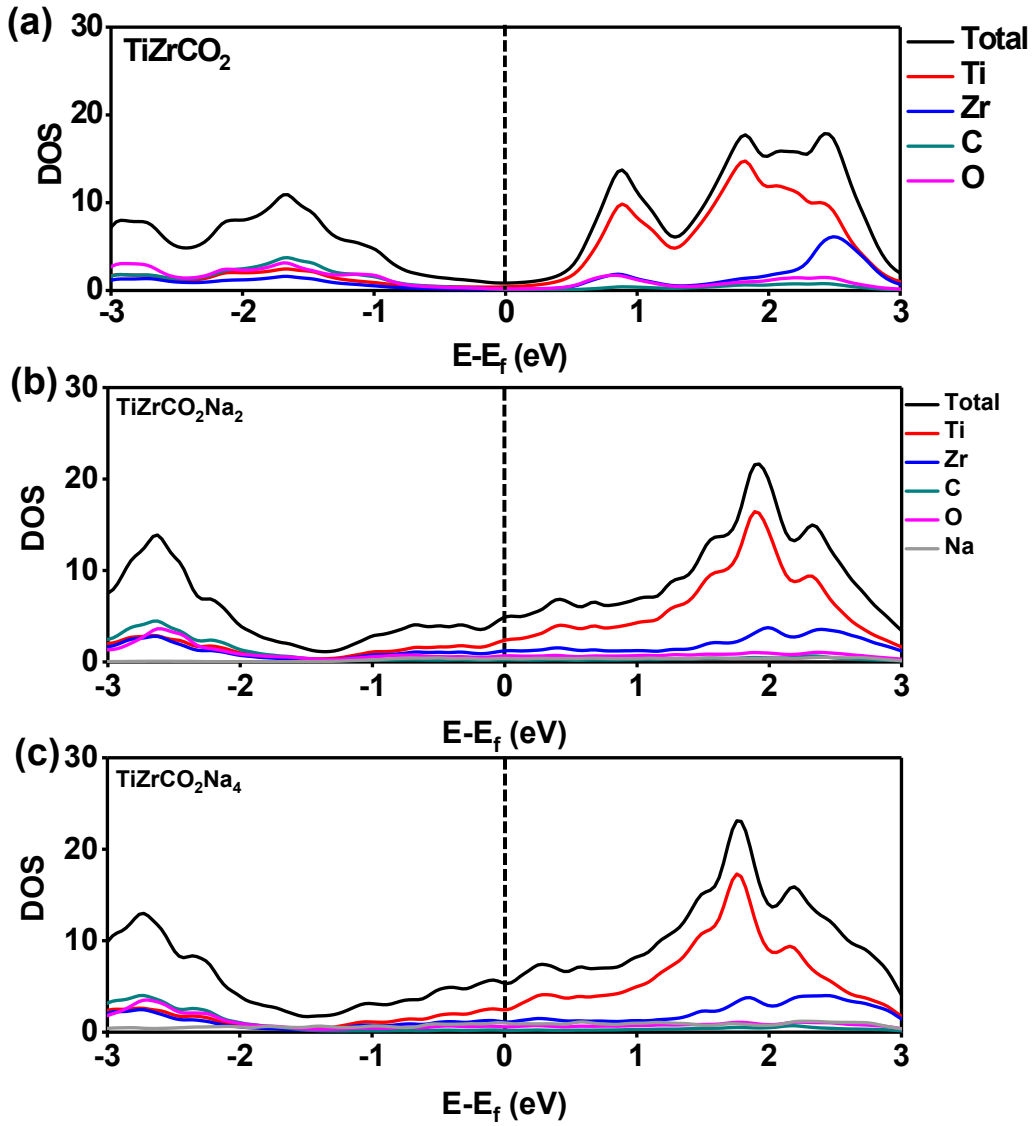


**Figure S2.** Density of states (DOS) of $TiZrCO_2$ (a), $TiZrCO_2Na_2$ (b) and $TiZrCO_2Na_4$ (c). The Fermi level is set to zero, which is shown at the black dotted line.

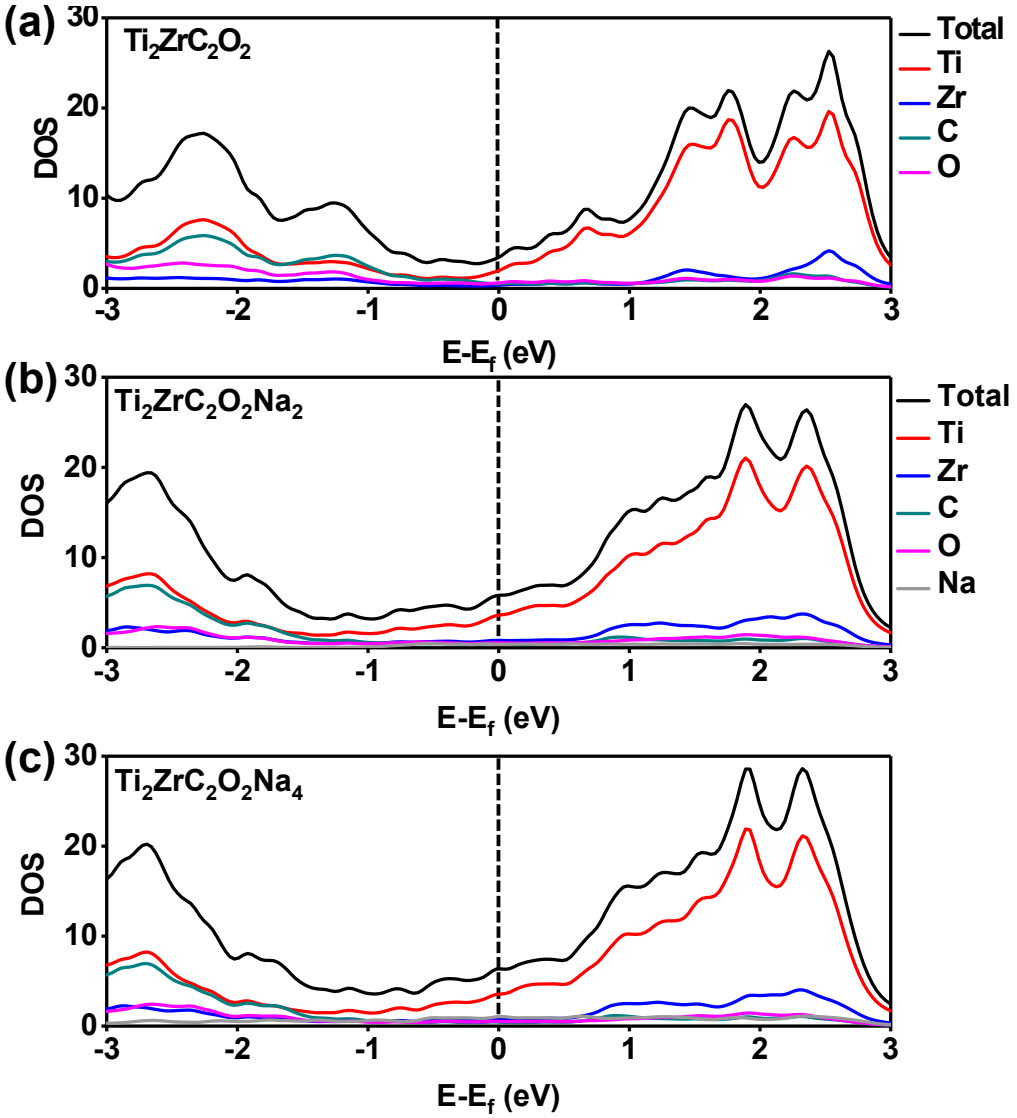


**Figure S3.** Density of states (DOS) of $Ti_2ZrC_2O_2$ (a), $Ti_2ZrC_2O_2Na_2$ (b) and $Ti_2ZrC_2O_2Na_4$ (c). The Fermi level is set to zero, which is shown at the black dotted line.

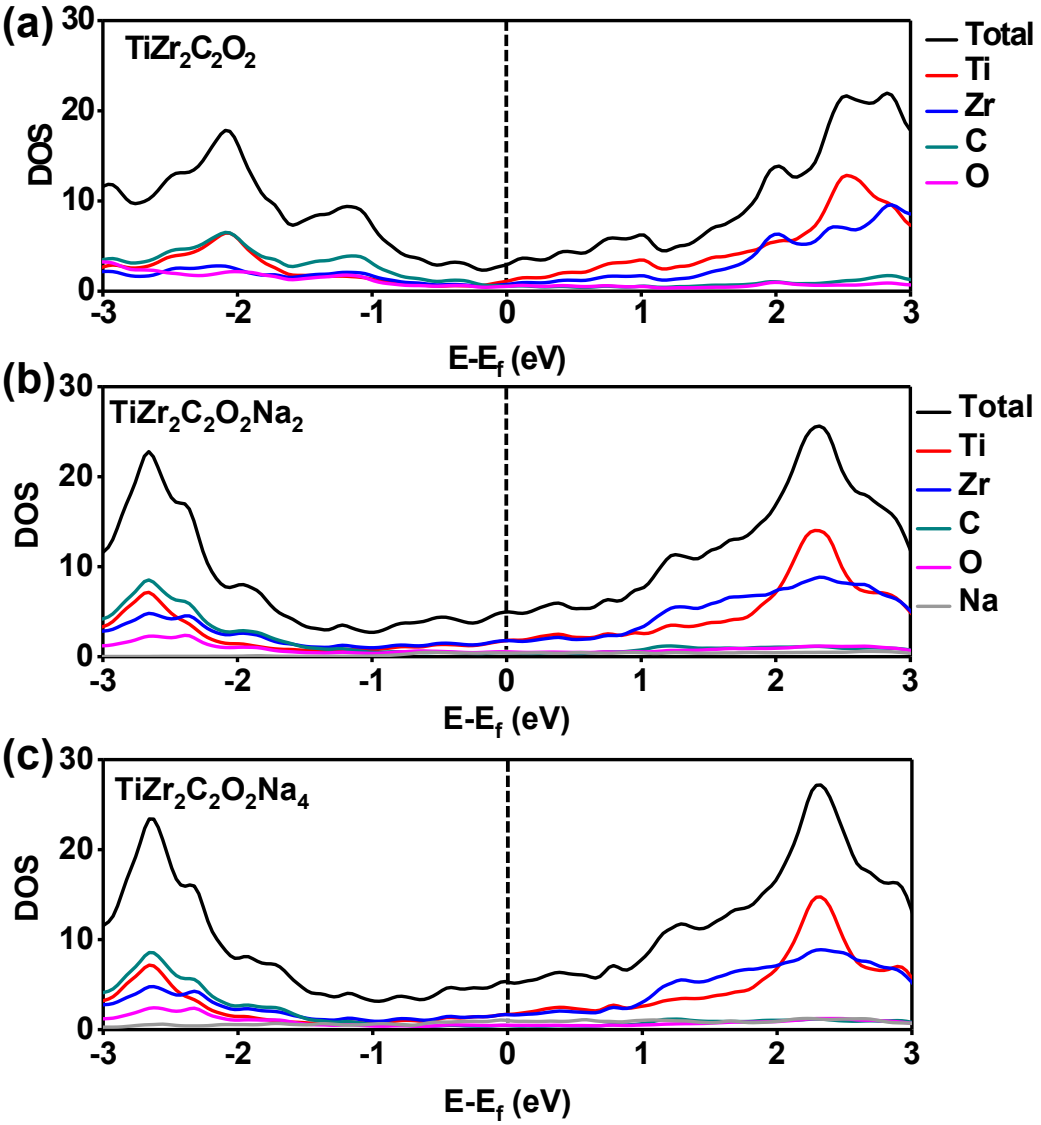


**Figure S4.** Density of states (DOS) of $TiZr_2C_2O_2$ (a), $TiZr_2C_2O_2Na_2$ (b) and $TiZr_2C_2O_2Na_4$ (c). The Fermi level is set to zero, which is shown at the black dotted line.

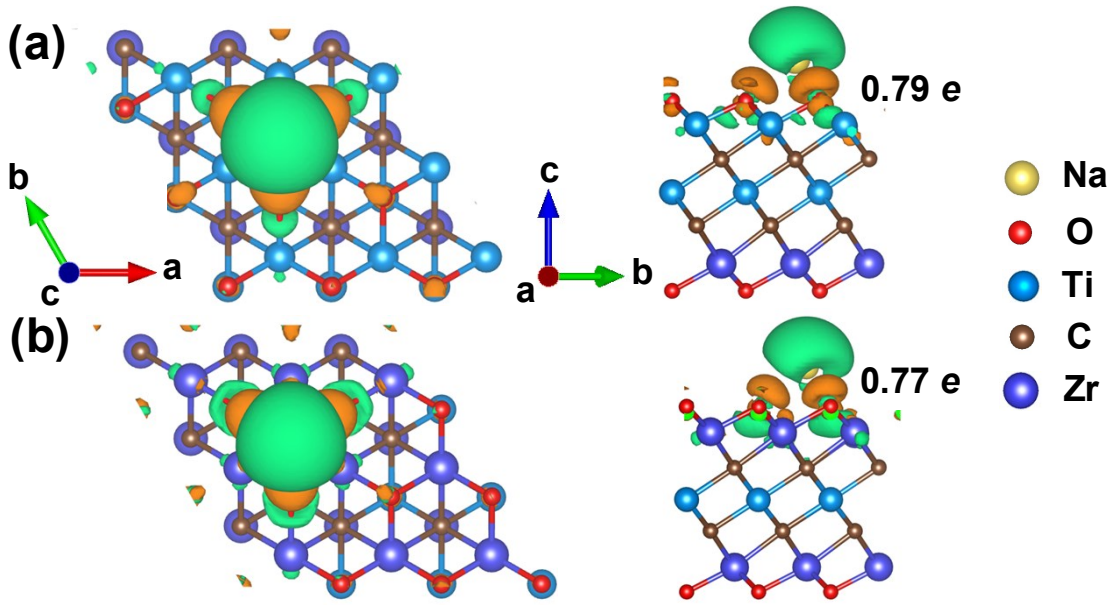


**Figure S5.** Charge density difference during adsorption process of the Na atom on $Ti_2ZrC_2O_2$ (a) and $TiZr_2C_2O_2$ (b) monolayer in top and side views. The isosurface level is set to be 0.01 e/Å$^3$. Green and orange regions indicate electron depletion and accumulation, respectively.

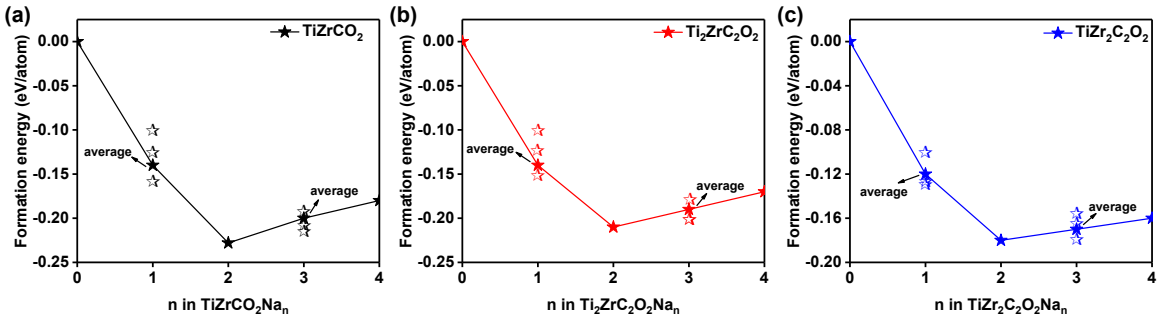


**Figure S6**. Formation energies of (a) $TiZrCO_2Na_n$, (b) $Ti_2ZrC_2O_2Na_n$, and (c) $TiZr_2C_2O_2Na_n$ at 0 K. For n = 1 and 3, solid pentagram refers to the average value, while hollow pentagram refers to the true value.

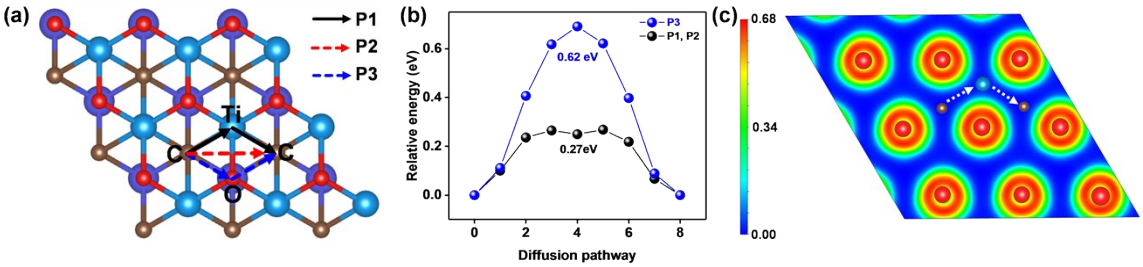


**Figure S7.** Potential diffusion pathways (a), corresponding diffusion energy barriers of Na atom on $TiZrCO_2$ monolayer (b) and electron localization function of (001) section for $TiZrCO_2$ (c).

**Table S1.** The calculated adsorption energies (eV) of single Na atom on three potential sites of $TiZrCO_2$

| Site | A | B | C |
|---|---|---|---|
| $E_{ads}$(eV) | -1.26 | -0.82 | -1.50 |

**Table S2.** Summary of the sequential adsorption energies, $E_{ads}$ (eV/atom), of the second layer Na atoms on $TiZrCO_2$ and $Ti_2ZrC_2O_2$

| Systems | Sequential $E_{ads}$ of the 2nd layer Na atoms | | | |
|---|---|---|---|---|
| | 1st Ti_side | 2nd Zr_side | 1st Zr_side | 2nd Ti_side |
| $TiZrCO_2$ | - 0.01 | - 0.03 | - 0.03 | - 0.01 |
| $Ti_2ZrC_2O_2$ | - 0.01 | - 0.02 | - 0.02 | - 0.01 |