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Modelling high performance potassium-ion batteries anode materials with two-dimensional vanadium carbide MXene: The role of surface O- and S-terminations

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Figure S1. (a) Top and side view of snapshot after equilibration and (b) free energy as a function of MD time at the temperature of 300 K for $V_2CO_2K_{2.67}$.



Figure S2. (a) Top and side view of snapshot after equilibration and (b) free energy as a function of MD time at the temperature of 300 K for $V_2CS_2K_{1.33}$.