Electronic supplementary information (ESI)

New Family of Layered N-Based Cathode Materials for Sodium-Ion Batteries

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Supplementary Figures

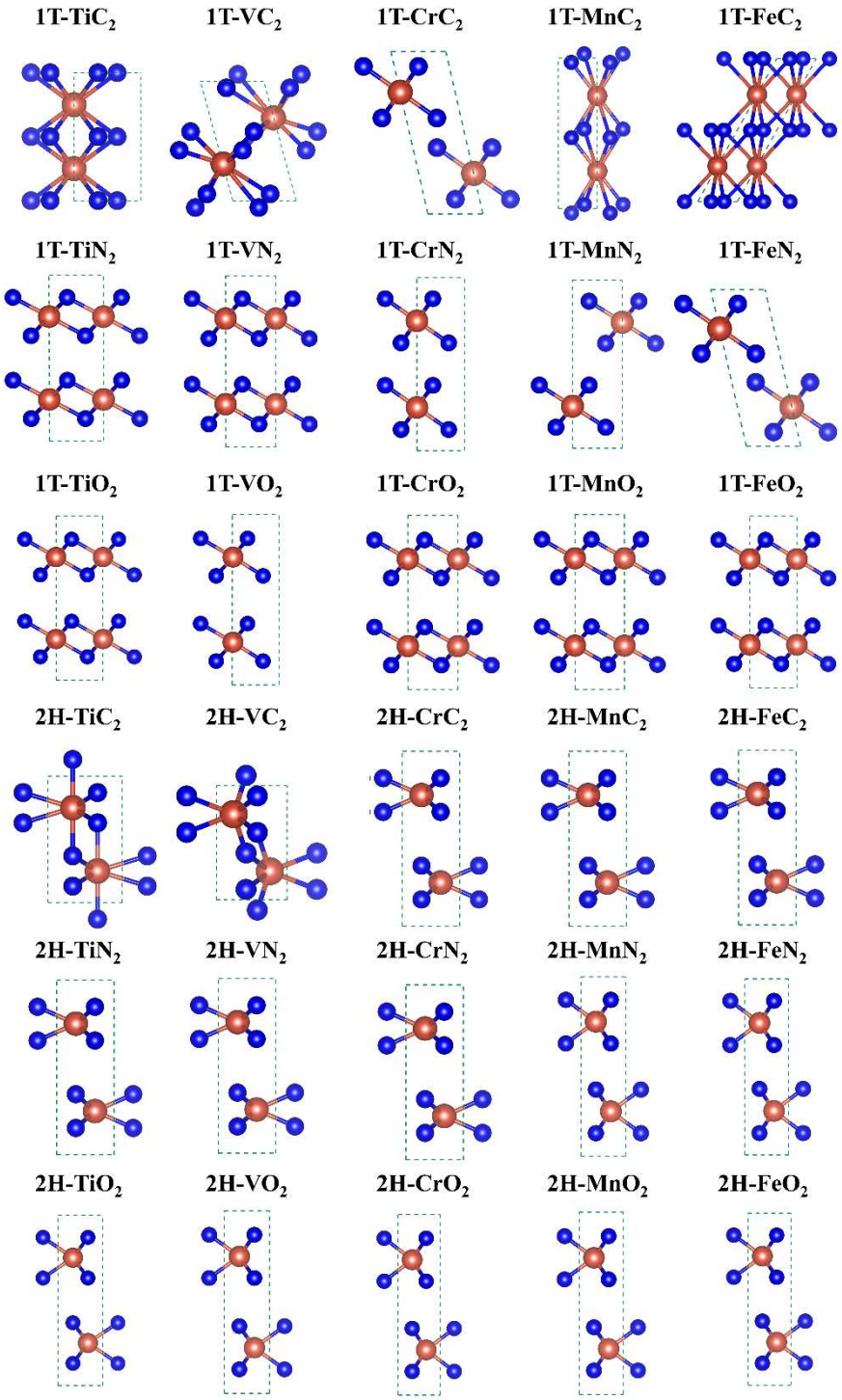

Fig. S1 The fully optimized structures of 1T- and 2H-phase MX_2 (M=Ti, V, Cr, Mn and Fe; X=C, N and O). (Brown and blue balls represent M and X atoms, respectively).

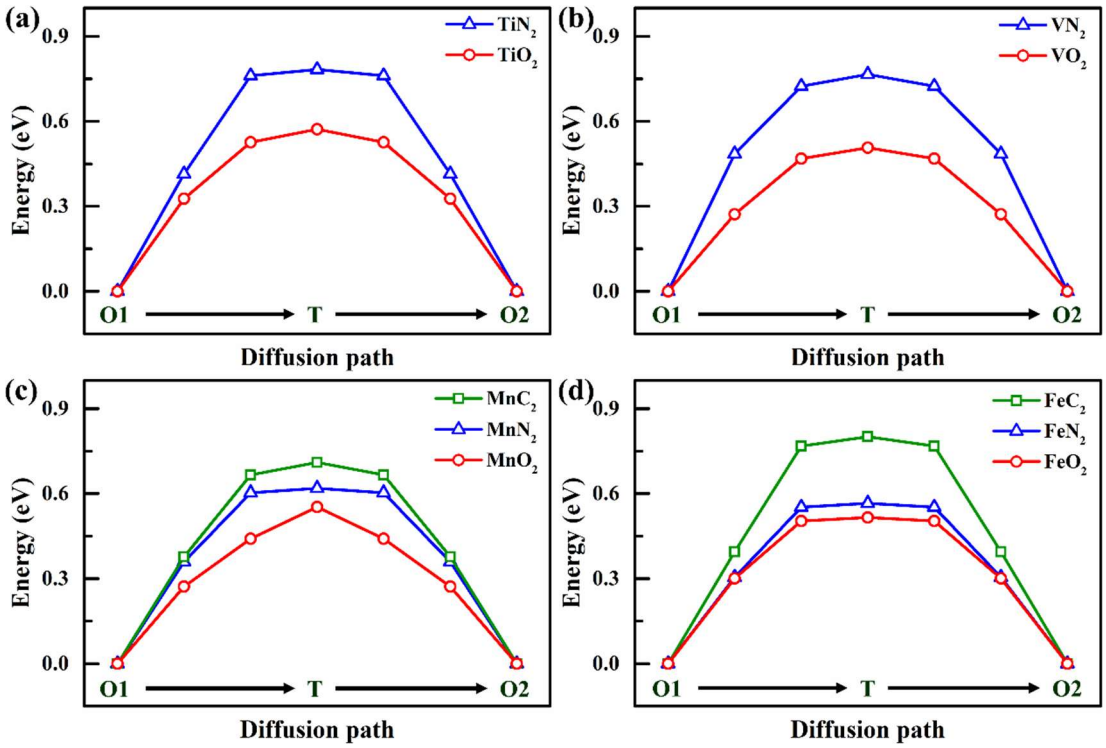

Fig. S2 Energy profile of Na diffusing along the diffusion path in 2H-phase MX_2 (M=Ti, V, Mn and Fe; X=C, N and O).

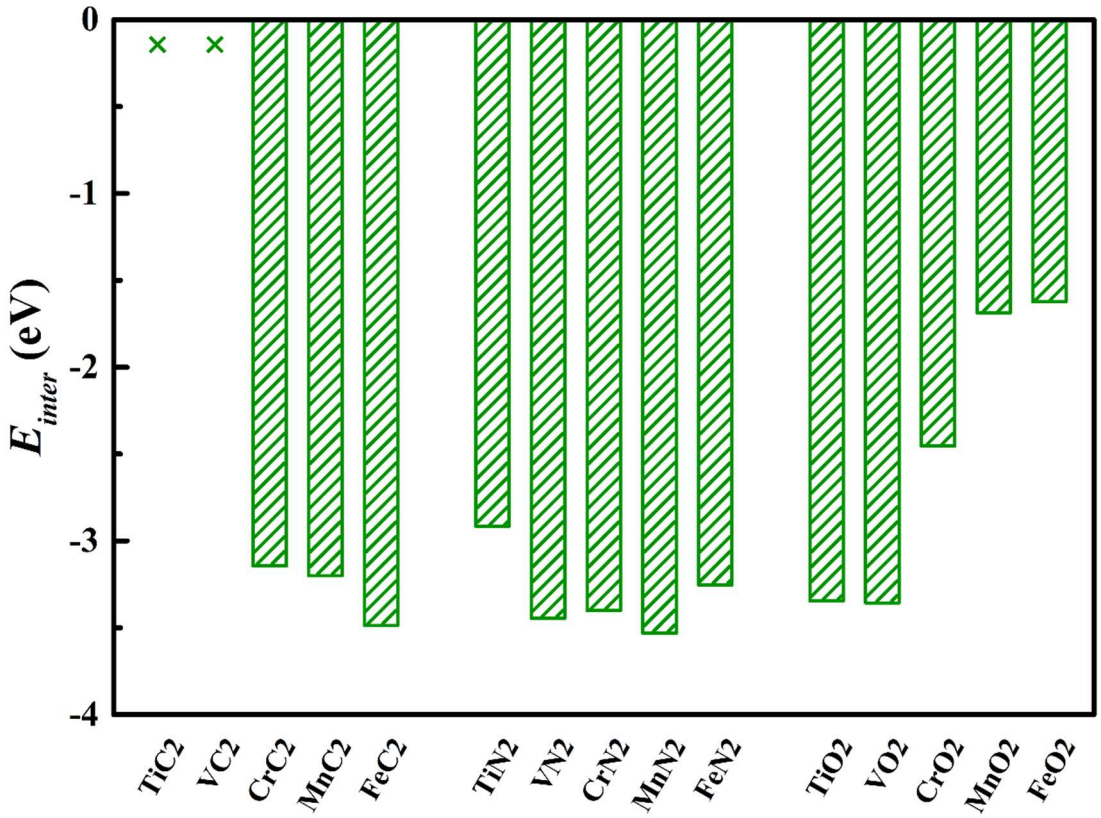

Fig. S3 The intercalation energy for Na intercalated in 2H-phase MX2 (M=Ti, V, Cr, Mn and Fe; X=C, N and O). (Note: The intercalation energy E_{inter} is defined as $E_{inter} = E_{NaMX2} - E_{MX} - \mu_{Na}$, here the E_{NaMX2} and E_{MX2} represent the total energy of $NaMX_2$ and MX_2 respectively, and the μ_{Na} is the chemical potential of Na atom.)

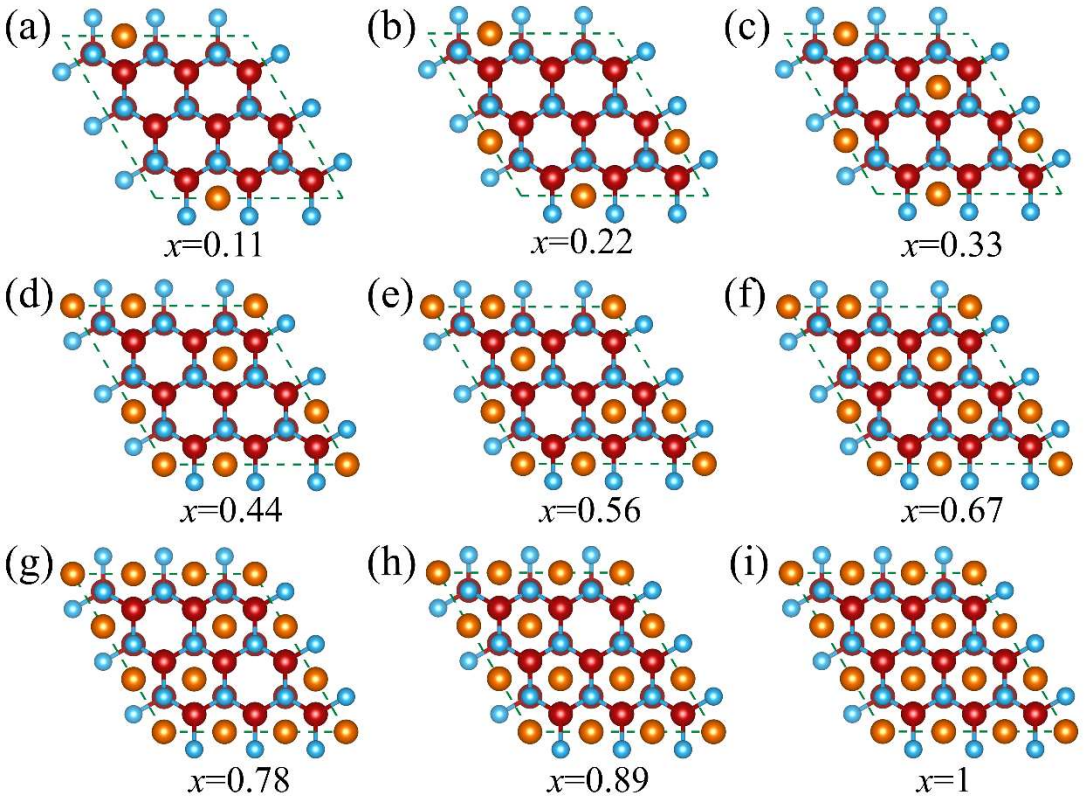

Fig. S4 The most stable configuration of Na_xCrN_2 (x = 0 ~ 1) under different sodium concentrations. (Light brown balls, dark red balls and light blue balls represent sodium, chromium, and nitrogen, respectively).

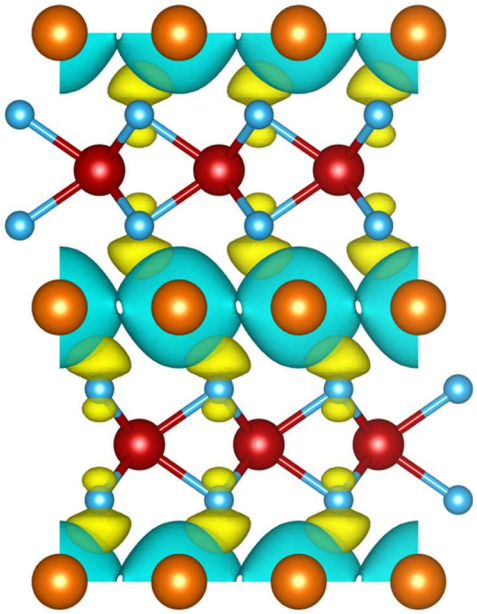

Fig. S5 Differential charge density of $NaCrN_2$. (Light brown balls, dark red balls, and light blue balls represent sodium, chromium, and nitrogen, respectively. Yellow areas and cyan areas represent electron-rich regions and electron-deficient regions, respectively. Isosurface level is set to 0.01 e/Å^3).

Supplementary Tables

Table S1 Calculated lattice parameters of all MX_2 structures (M=Ti, V, Cr, Mn and Fe; X=C, N and O).

		C		N		O	
		1T	2H	1T	2H	1T	2H
Ti	*a* (Å)	3.04	3.75	3.10	3.19	2.98	2.89
	c (Å)	5.70	5.53	8.19	8.13	9.02	9.51
V	*a* (Å)	3.50	4.12	2.89	3.08	2.90	2.74
	c (Å)	6.22	4.53	8.55	8.06	9.09	9.59
Cr	*a* (Å)	2.69	3.06	2.72	3.08	2.89	2.62
	c (Å)	8.19	8.63	8.57	8.13	8.73	9.74
Mn	*a* (Å)	2.46	3.02	2.79	2.65	2.88	2.65
	c (Å)	8.30	8.19	8.16	9.15	8.81	9.53
Fe	*a* (Å)	2.54	2.97	2.81	2.61	2.80	2.68
	c (Å)	9.37	8.34	7.73	9.11	8.85	9.32

Table S2 Lattice constant *a* and layer thickness *h* of VN_2.

		a (Å)	*h* (Å)
VN_2	Our	3.08	1.57
	Other[43]	3.10	1.55

Note: Ref. 43 was cited in main article.

43 Y. Dong, Z. Tang, P. Liang, H. Wan, H. Wang, L. Wang, H. Shu and D. Chao, *J. Colloid Interf. Sci.*, 2021, **593**, 51-58.

Table S3 Relaxed atomic positions for 2H-phase CrN_2 whose space group is $P6_3/mmc$.

Atom	*x*	*y*	*z*
Cr 1	0.333	0.666	0.250
Cr 2	0.666	0.333	0.750
N 1	0.666	0.333	0.158
N 2	0.666	0.333	0.342
N 3	0.333	0.666	0.658
N 4	0.333	0.666	0.842