Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Material

for

Carrier Transport in Bulk and Two-Dimensional $Zn_2(V, Nb, Ta)N_3$ Ternary Nitrides

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Table S1. The calculated elastic constants C_{ij} for bulk $Zn_2(V, Nb,Ta)N_3$.

Elastic constants	bulk Zn_2VN_3, GPa	bulk Zn_2NbN_3, GPa	bulk Zn_2TaN_3, GPa
C_{11}	235	217	219
C_{22}	239	210	210
C_{33}	258	221	231
C_{12}	105	99	96
C_{13}	114	112	112
C_{23}	103	95	95
C_{44}	59	52	54
C_{55}	55	49	51
C_{66}	52	52	53

Table S2. The Young modulus for 2D $Zn_2(V, Nb,Ta)N_3$.

Material	E_{xx}, N/m	E_{yy}, N/m
bulk Zn_2VN_3	109	108
bulk Zn_2NbN_3	87	95
bulk Zn_2TaN_3	88	88

Table S3. Cohesive energy for bulk and 2D $Zn_2(V, Nb,Ta)N_3$.

Structure	Cohesive energy, eV per atom
bulk Zn_2VN_3	-3.84
bulk Zn_2NbN_3	-4.11
bulk Zn_2TaN_3	-4.21
2D Zn_2VN_3	-3.60
2D Zn_2NbN_3	-3.82
2D Zn_2TaN_3	-3.91

Table S4. Calculated charge carrier effective mass (m_x^*, m_y^* and m_z^* in units of electron mass m_0), deformation potential (δ_x, δ_y, and δ_z, eV), mobility (μ_x, μ_y, and μ_z, $cm^2/V{\cdot}s$), and relaxation time (τ_x, τ_y and τ_z, ps) in bulk $Zn_2(V, Nb,Ta)N_3$ at T = 300 K.

Material	Reciprocal coordinate	m_x^*/m_0	m_y^*/m_0	m_z^*/m_0	δ_x	δ_y	δ_z	μ_x	μ_y	μ_z	τ_x	τ_y	τ_z
Zn_2VN_3	Electrons												
	(-0.500; 0.500; 0)	0.94	0.87	0.60	7.83	8.78	6.75	$2.73{\cdot}10^2$	$2.64{\cdot}10^2$	$1.26{\cdot}10^3$	0.15	0.13	0.43
	Holes												
	(0.314; 0.314; 0)	1.38	0.59	2.15	7.93	8.99	6.49	$1.02{\cdot}10^2$	$6.69{\cdot}10^2$	$0.55{\cdot}10^2$	0.08	0.23	0.07
Zn_2NbN_3	Electrons												
	(-0.500; 0.500; 0)	1.03	0.94	0.40	8.62	8.59	7.81	$1.65{\cdot}10^2$	$2.02{\cdot}10^2$	$2.20{\cdot}10^3$	0.10	0.11	0.50
	Holes												
	(-0.346; 0.653; 0)	3.86	0.87	1.88	8.98	9.60	8.26	$0.06{\cdot}10^2$	$1.97{\cdot}10^2$	$0.40{\cdot}10^2$	0.01	0.10	0.04
Zn_2TaN_3	Electrons												
	(-0.500; 0.500; 0)	1.15	1.12	0.43	7.31	6.23	5.68	$1.77{\cdot}10^2$	$2.47{\cdot}10^2$	$3.68{\cdot}10^3$	0.12	0.16	0.89
	Holes												
	(-0.335; 0.664; 0)	2.24	0.75	1.69	7.83	8.37	7.23	$0.29{\cdot}10^2$	$3.78{\cdot}10^2$	$0.73{\cdot}10^2$	0.04	0.16	0.07

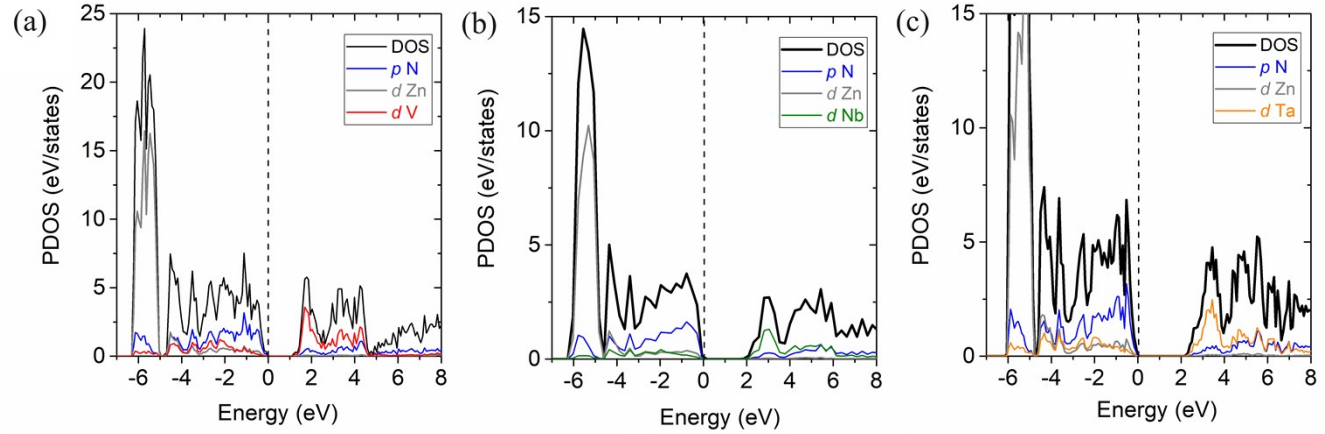

Figure S1. PDOS of bulk Zn_2VN_3 (a), Zn_2NbN_3 (b), and Zn_2TaN_3 (c).

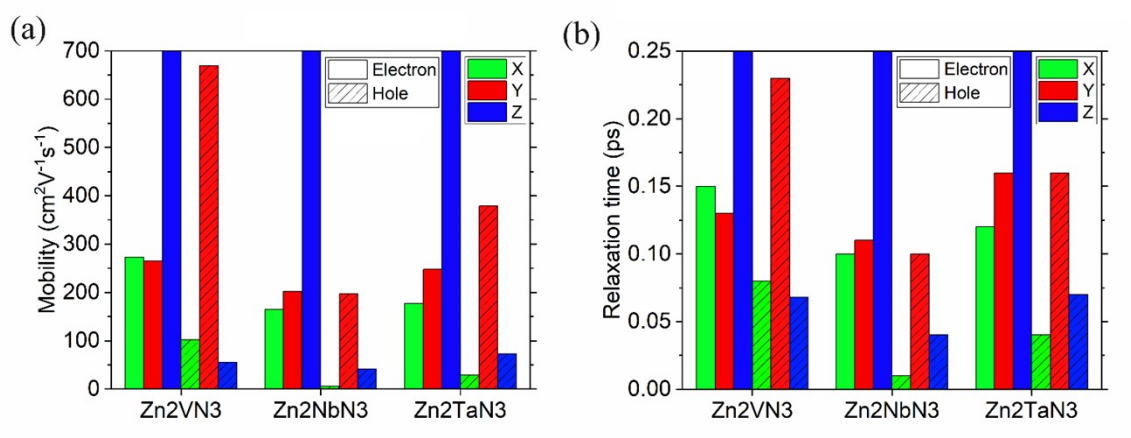

Figure S2. Magnified plots for charge mobility (μ) (a) and relaxation time (τ) (b) for holes and electrons in bulk $Zn_2(V, Nb,Ta)N_3$.

Table S5. Calculated charge carrier effective mass (m_x^*, m_y^* and m_z^* in units of electron mass m_0), deformation potential (δ_x, δ_y, δ_z, eV), mobility (μ_x, μ_y, and μ_z, $cm^2/V \cdot s$), and relaxation time (τ_x, τ_y and τ_z, ps) in 2D $Zn_2(V, Nb,Ta)N_3$ at T = 300 K.

Material	Reciprocal coordinate	m_x^*/m_0	m_y^*/m_0	δ_x	δ_y	μ_x	μ_y	τ_x	τ_y
Zn_2VN_3	Electrons								
	(0; 0; 0)	2.15	4.07	1.67	4.00	$1.30 \cdot 10^2$	$0.12 \cdot 10^2$	0.16	0.03
	Holes								
	(-0.255; 0.255; 0)	2.55	2.31	-0.92	1.75	$0.44 \cdot 10^3$	$1.33 \cdot 10^2$	0.63	0.17
Zn_2NbN_3	Electrons								
	(-0.500; 0.500; 0)	1.01	2.15	0.27	0.80	$1.67 \cdot 10^4$	$0.99 \cdot 10^3$	9.60	1.21
	Holes								
	(-0.216; 0.216; 0)	2.06	1.63	1.78	2.31	$1.56 \cdot 10^2$	$1.27 \cdot 10^2$	0.18	0.12
Zn_2TaN_3	Electrons								
	(-0.500; 0.500; 0)	0.88	2.39	-1.53	0.57	$0.63 \cdot 10^3$	$1.67 \cdot 10^3$	0.31	2.27
	Holes								
	(-0.167; 0.167; 0)	2.16	2.95	1.00	2.30	$3.41 \cdot 10^2$	$0.47 \cdot 10^2$	0.42	0.08

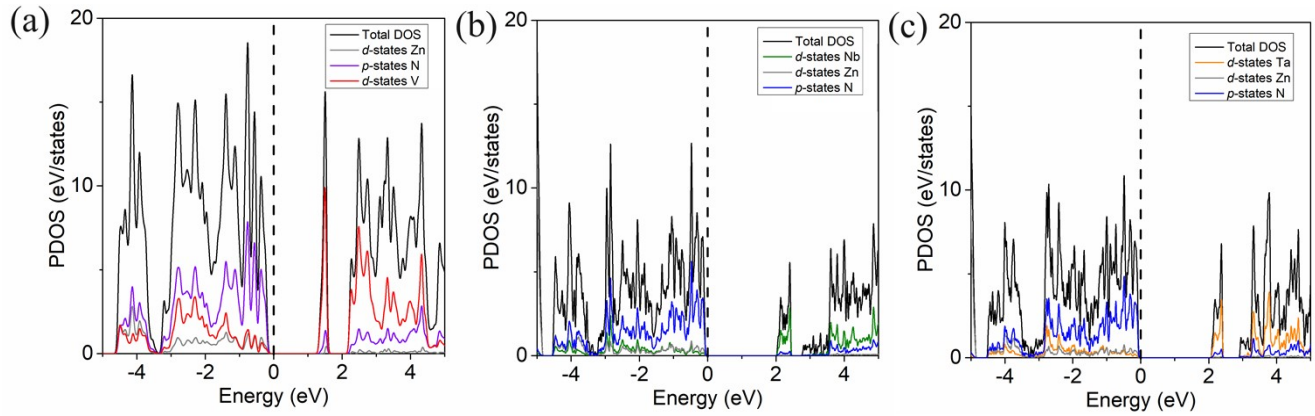

Figure S3. PDOS of 2D Zn_2VN_3 (a), 2D Zn_2NbN_3 (b), and 2D Zn_2TaN_3 (c).

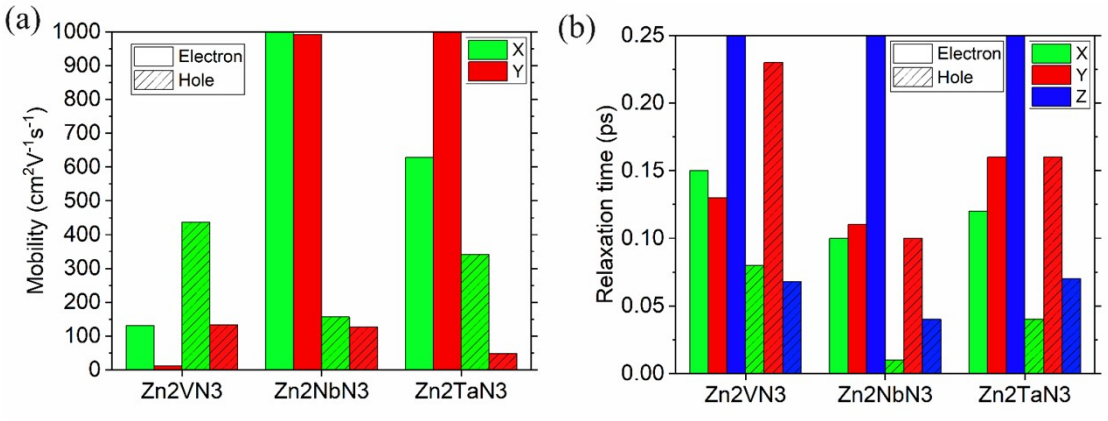

Figure S4. Magnified charge mobility (μ) (a) and relaxation time (τ) (b) for holes and electrons in 2D $Zn_2(V, Nb,Ta)N_3$.

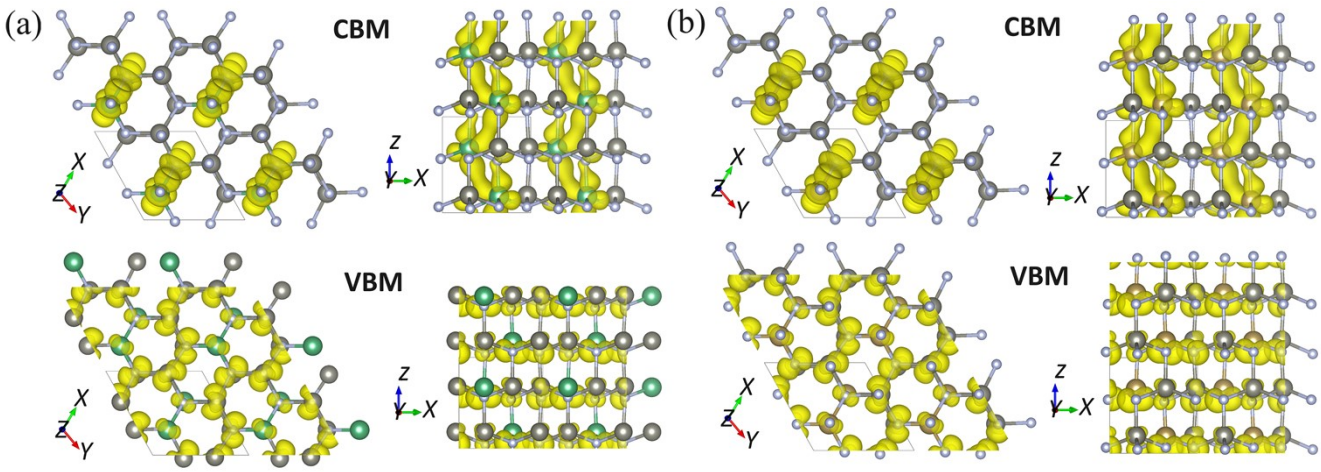

Figure S5. Top and side views of the spatial structure of wave functions in VBM and CBM for bulk Zn_2NbN_3 (a) and Zn_2TaN_3 (b) at the *k* points corresponding to VBM and CBM, respectively (Table S4). The isosurface of 0.003 e Å^{-3} is adopted.

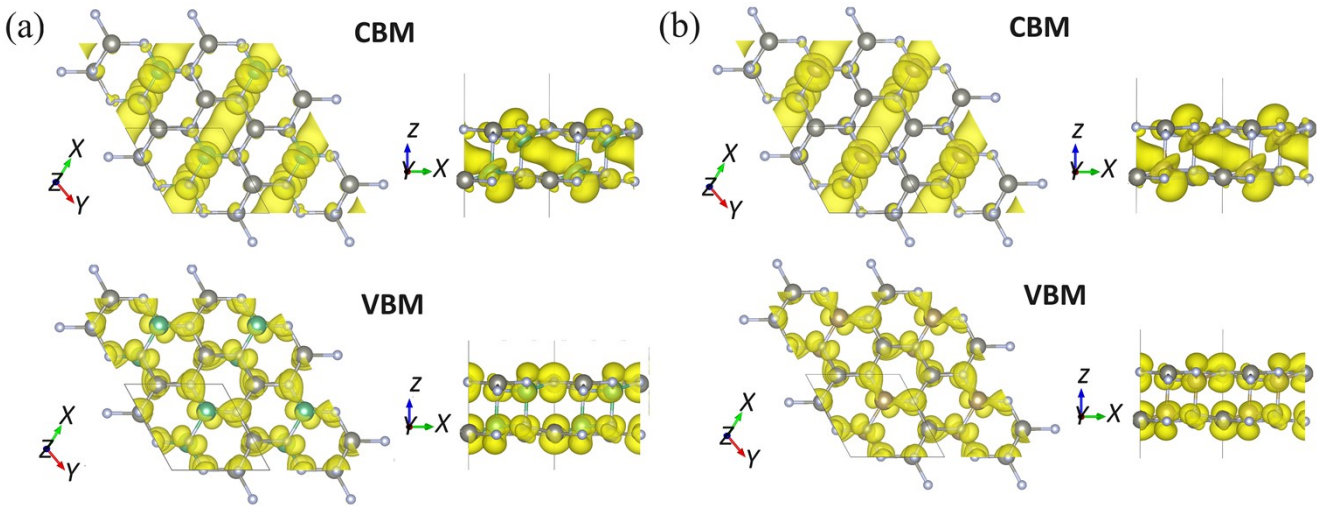

Figure S6. Top and side views of the spatial structure of wave functions in VBM and CBM for 2D Zn_2NbN_3 (a) and 2D Zn_2TaN_3 (b) at the *k* points corresponding to VBM and CBM, respectively (Table S5). The isosurface of 0.003 e Å^{-3} is adopted.