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Ultrahigh conductivity and non-trivial band structure in van der Waals Nb dichalcogenides with Ge intercalation

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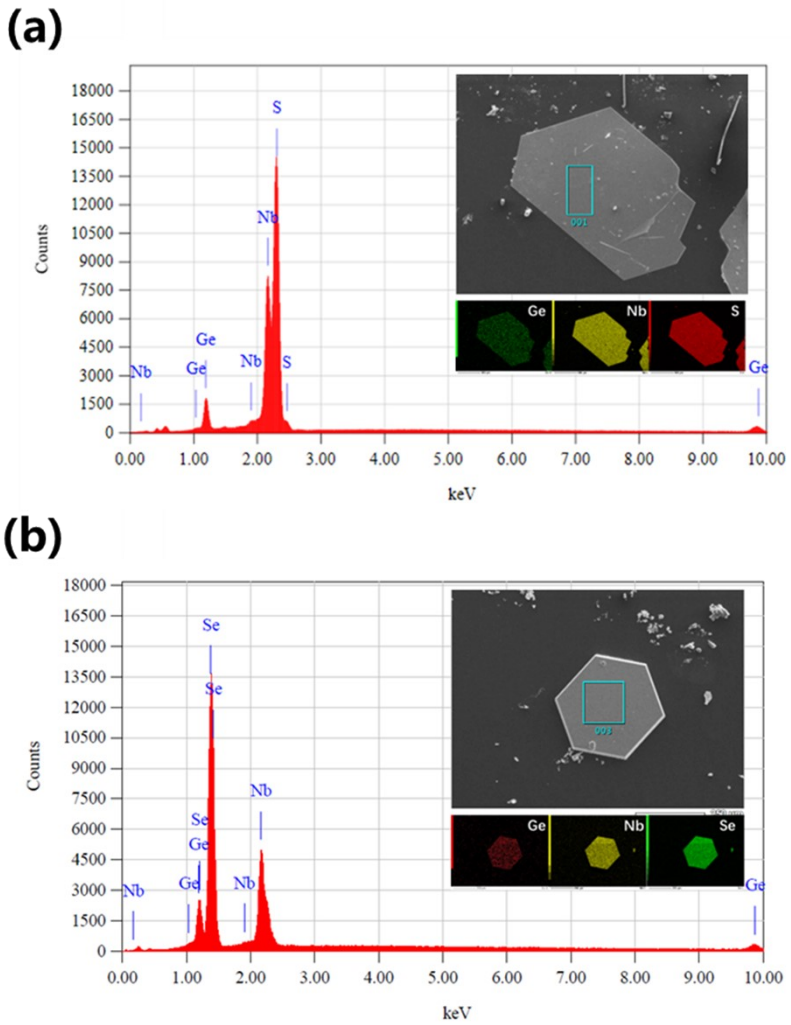

Figure S1. The SEM images, EDS and elemental mapping results of (a) $Ge_{0.33}NbS_2$ and (b) $Ge_{0.26}NbSe_2$.

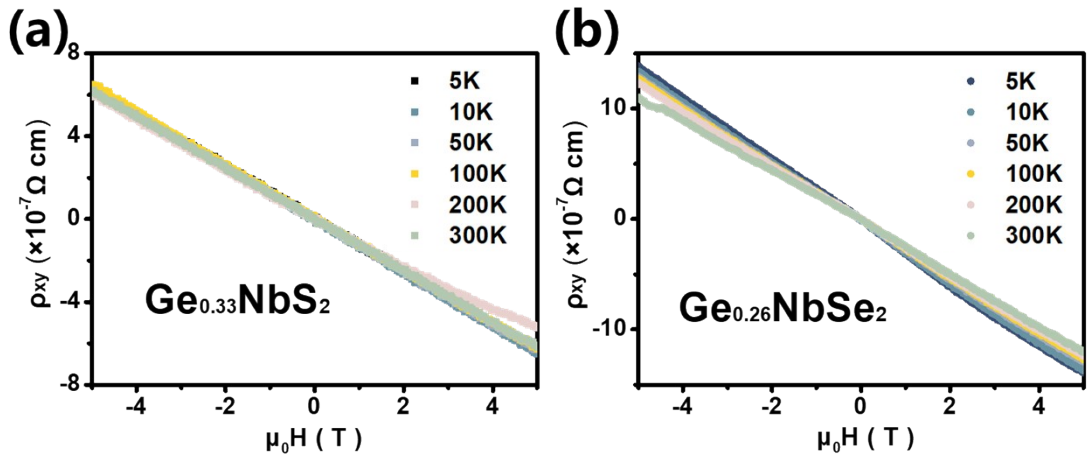

Figure S2. Magnetic field dependence of the Hall resistivity of (a) $Ge_{0.33}NbS_2$ and (b) $Ge_{0.26}NbSe_2$ single crystals.

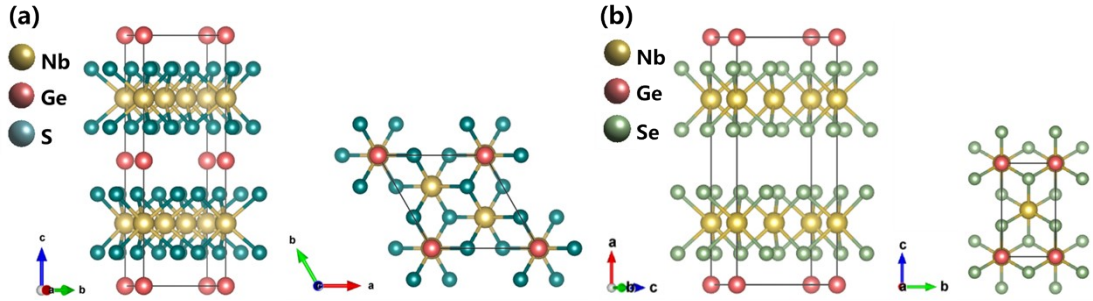

Figure S3. The structure models of (a) $Ge_{0.33}NbS_2$ and (b) $Ge_{0.26}NbSe_2$ used for calculation. Two different types of superlattice were used to simulate the different Ge configurations in $Ge_{0.33}NbS_2$ and $Ge_{0.26}NbSe_2$.

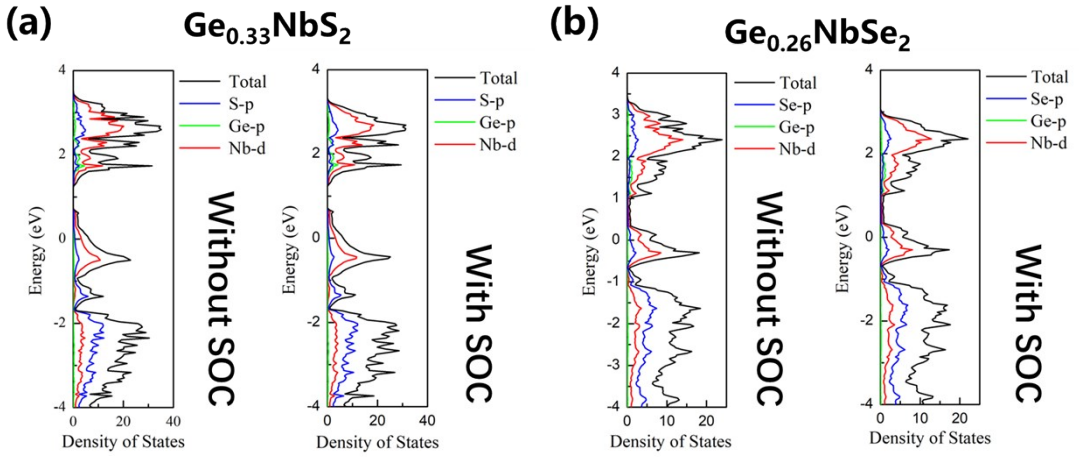

Figure S4. (a) The partial DOS for $Ge_{0.33}NbS_2$ with/without SOC; (b) The partial DOS for $Ge_{0.26}NbSe_2$ with/without SOC.

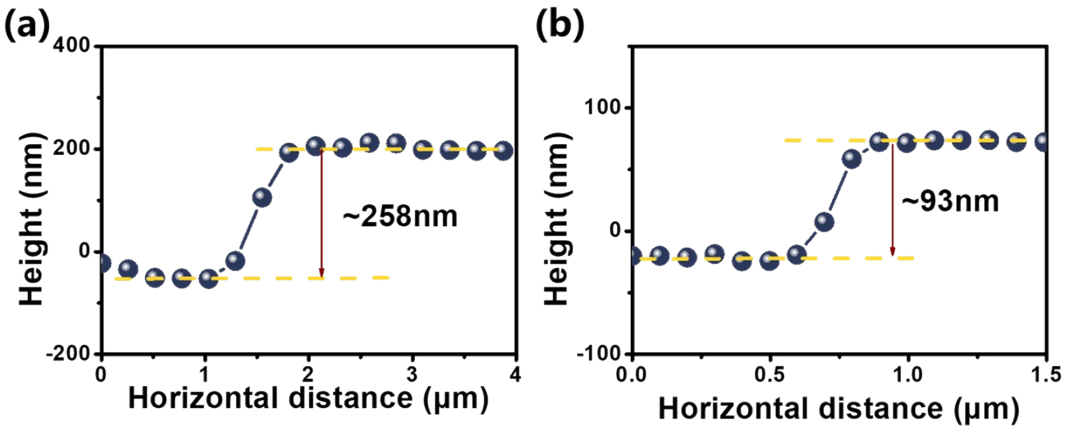

Figure S5. (a) The corresponding height value of the white dotted line in Figure 6a; (b) The corresponding height value of the white dotted line in Figure 6b.

Table S1. Crystallographic Data and Structure Refinement of $Ge_{0.33}NbS_2$.

Empirical formula	$Ge_{0.33}NbS_2$
Formula weight	181.23
Crystal system	hexagonal
Space group	$P6_3/mcm$
Unit cell dimensions	a=5.756(2) Å, α=90 °
	b=5.756(2) Å, β=90 °
	c=13.474(4) Å, γ=120 °
Volume, Z	386.6 (2) $Å^3$, 6
Density (calculated)	4.671 g/cm^3
2θ range for data collection	6.05° to 56.68°
Index ranges	$-7 \leq h \leq 7, -6 \leq k \leq 7, -17 \leq l \leq 18$
Reflections collected	3097
Independent reflections	201 [R_{int} = 0.0921, R_{sigma} = 0.0567]
Data/restraints/parameters	201/0/13
Goodness-of-fit on F^2	1.340
Final R indexes [I≥2σ(I)]	R_1 = 0.0584, wR_2 = 0.1084
Final R indexes [all data]	R_1 = 0.0615, wR_2 = 0.1137
Largest diff. peak and hole	1.81/-7.08 e·$Å^{-3}$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Ge_{0.33}NbS_2$ estimated standard deviations in parentheses.

Label	***x***	***y***	***z***	**Occupancy**	U_{eq}^*
Nb(1)	0	0	2500	1.00	2(1)
Nb(2)	-3333.33	3333.33	2500	1.00	2(1)
S	-3356(2)	0	1335.2(10)	1.00	3(1)
Ge	0	0	0	1.00	7(1)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Ge_{0.33}NbS_2$ with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb(1)	2(1)	2(1)	2(1)	0	0	1(1)
Nb(2)	2(1)	2(1)	2(1)	0	0	1(1)
S	3(1)	3(1)	3(1)	0	0(1)	2(1)
Ge	6(1)	6(1)	10 (1)	0	0	3(1)

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S4. Crystallographic Data and Structure Refinement of $Ge_{0.26}NbSe_2$.

Empirical formula	$Ge_{0.26}NbSe_2$
Formula weight	269.34
Crystal system	hexagonal
Space group	$P6_3/mmc$
Unit cell dimensions	a=3.454(6) Å, α=90 °
	b=3.454(6) Å, β=90 °
	c=13.480(4) Å, γ=120 °
Volume, Z	139.93(7) $Å^3$, 2
Density (calculated)	6.421 g/cm^3
2θ range for data collection	6.04° to 54.94°
Index ranges	$-4 \le h \le 2$, $-4 \le k \le 4$, $-17 \le l \le 16$
Reflections collected	1020
Independent reflections	85 [R_{int} = 0.0575, R_{sigma} = 0.0273]
Data/restraints/parameters	85/0/9
Goodness-of-fit on F^2	1.405
Final R indexes [I≥2σ(I)]	R_1 = 0.0699, wR_2 = 0.1773
Final R indexes [all data]	R_1 = 0.0705, wR_2 = 0.1781
Largest diff. peak and hole	2.19/-3.24 $e \cdot Å^{-3}$

Table S5. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Ge_{0.26}NbSe_2$ estimated standard deviations in parentheses.

Label	*x*	*y*	*z*	Occupancy	U_{eq}^*
Se	3333.33	6666.67	3738(4)	1.00	29(2)
Nb	0	10000	2500	1.00	28 (2)
Ge	0	10000	5000	0.26(3)	26(9)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S6. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Ge_{0.33}NbS_2$ with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Se	21(2)	21(2)	45(3)	0	0	10(1)
Nb	20(2)	20(2)	44(4)	0	0	10(1)
Ge	29(11)	29(11)	19(13)	0	0	15(5)

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S7. The conductivities of different materials at room temperature in Figure 3c.

Material	Conductivity ($S \cdot cm^{-1}$)
$Ge_{0.33}NbS_2$	6.83×10^4
$Ge_{0.26}NbSe_2$	5.48×10^3
NbS_2	9.09×10^3
TaS_2	8.33×10^3
VSe_2	3.03×10^3
$NbSe_2$	2.86×10^3
$TaSe_2$	2.50×10^3
$PtSe_2$	7.69×10^3
VTe_2	5.88×10^3
$NbTe_2$	3.85×10^3
$TaTe_2$	2.78×10^3
WTe_2	3.57×10^2
$PtTe_2$	4.17×10^4
Bi*	8.00×10^3
Ag*	6.21×10^5
Au*	4.55×10^5
Pt*	9.60×10^4

*The conductivities of Bi, Ag, Au and Pt were taken from G. T. Meaden, Electrical resistance of metals, Springer, 2013.