Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supplementary Information

Impurity States in $Mo_{1-x}M_xSe_2$ Compounds Doped with Group VB Elements and their Electronic and Thermal Transport Properties

Cheng Zhang, ‡[a] Zhi Li, ‡[a] Min Zhang,[a] Hongyao Xie,[a] Changhua Hong,[a] Xianli Su,[a] Gangjian Tan,[a] Pierre Ferdinand Poudeu Poudeu,[b] Ctirad Uher,[c] Wei Liu*[a] and Xinfeng Tang*[a]

[a] *State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan 430070, China. E-mail: w.liu@whut.edu.cn; tangxf@whut.edu.cn*

[b] *Materials Science and Engineering Department, University of Michigan, Ann Arbor, Michigan 48109, United States.*

[c] *Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, United States.*

‡ *C. Zhang and Z. Li contributed equally to this work.*

Table S1. Optimized lattice parameters of $Mo_{16}Se_{32}$ and $Mo_{15}MSe_{32}$ (M = V, Nb and Ta) based on the DFT.

	Compounds	*a*, *b* (Å)	*c* (Å)	Relative variation ratio	
				a, *b* (%)	*c* (%)
Calculations	$Mo_{16}Se_{32}$	3.29088	12.97660	/	/
	$Mo_{15}VSe_{32}$	3.29600	12.90482	0.16	–0.55
	$Mo_{15}NbSe_{32}$	3.30419	12.90731	0.40	–0.53
	$Mo_{15}TaSe_{32}$	3.30436	12.91242	0.41	–0.49

Table S2. Room temperature physical parameters of $Mo_{1-x}V_xSe_2$ ($0 < x \leq 0.09$).

Sample	*p* (10^{20} cm^{-3})	*μ* (cm^{2}V^{-1}s^{-1})	*σ* (10^4 Sm^{-1})	*S* (μVK^{-1})	*PF* (mWm^{-1}K^{-2})	m^*/m_0	κ_L (Wm^{-1}K^{-1})
$x = 0.01$	0.25	5.1	0.20	316	0.20	1.34	11.6
$x = 0.03$	2.3	3.4	1.24	101	0.13	1.88	10.0
$x = 0.05$	4.8	3.6	2.80	71	0.14	2.17	9.3
$x = 0.07$	5.6	3.0	2.71	67	0.12	2.24	8.9
$x = 0.09$	7.2	3.1	3.60	57	0.12	2.28	8.8

Table S3. Room temperature physical parameters of $Mo_{1-x}Nb_xSe_2$ ($0 < x \leq 0.09$).

Sample	*p* (10^{20} cm^{-3})	*μ* (cm^{2}V^{-1}s^{-1})	*σ* (10^4 Sm^{-1})	*S* (μVK^{-1})	*PF* (mWm^{-1}K^{-2})	m^*/m_0	κ_L (Wm^{-1}K^{-1})
$x = 0.01$	0.56	4.3	0.38	202	0.16	1.47	10.0
$x = 0.03$	3.6	3.9	2.24	91.5	0.19	2.29	9.6
$x = 0.05$	6.5	4.2	4.37	70.8	0.22	2.48	10.0
$x = 0.07$	9.1	4.0	5.80	56.9	0.19	2.65	8.4
$x = 0.09$	12.0	3.7	7.05	48.6	0.17	2.73	7.5

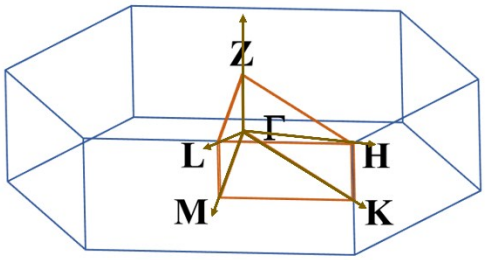

Fig. S1 The first Brillouin zone of MoQ_2 with high symmetry paths indicated.

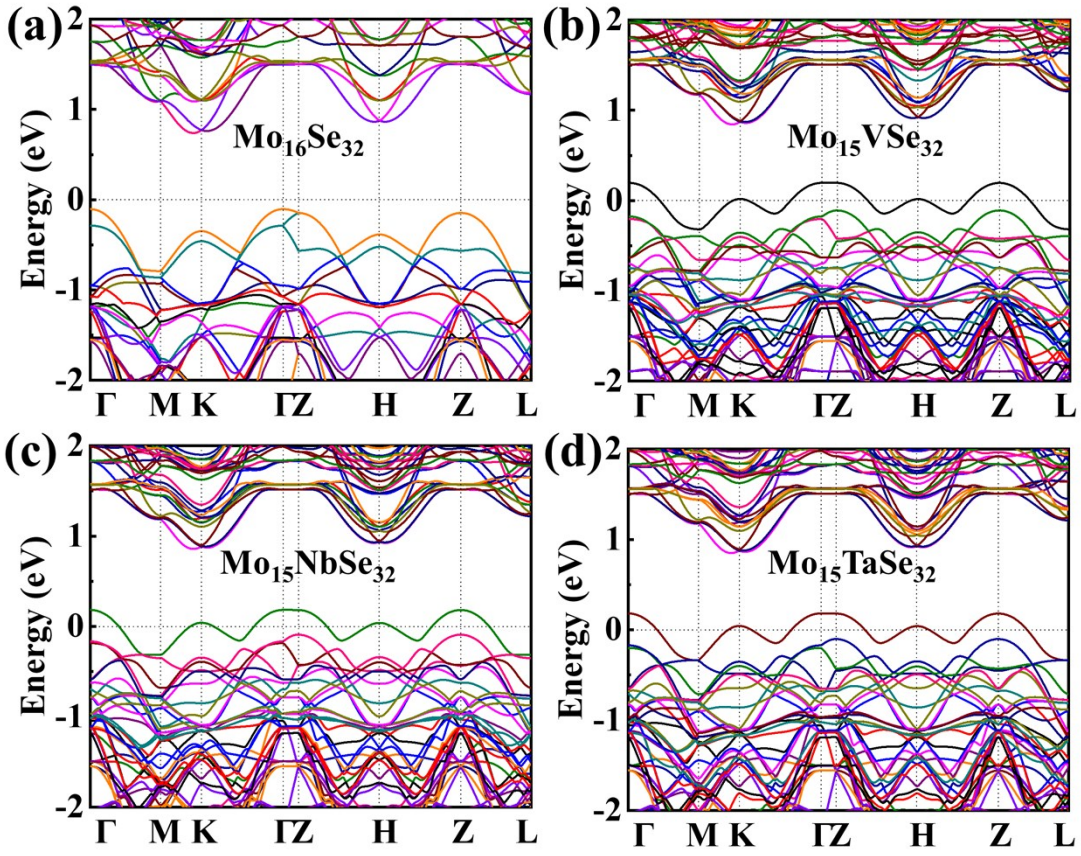

Fig. S2 Band structure of (a) $Mo_{16}Se_{32}$, (b) $Mo_{15}VSe_{32}$, (c) $Mo_{15}NbSe_{32}$, and (d) $Mo_{15}TaSe_{32}$ without SOC.

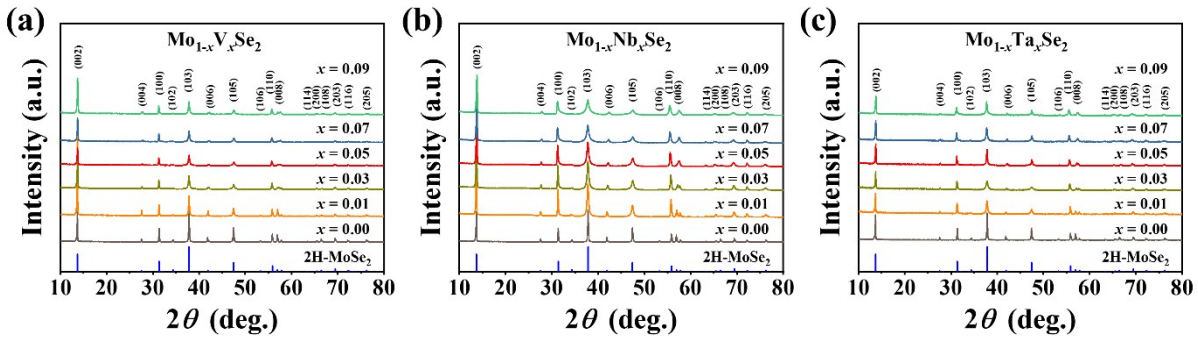

Fig. S3 Powder XRD pattern of $Mo_{1-x}M_xSe_2$ ($0 < x \leq 0.09$) compounds, where (a) M = V, (b) M = Nb, and (c) M = Ta.

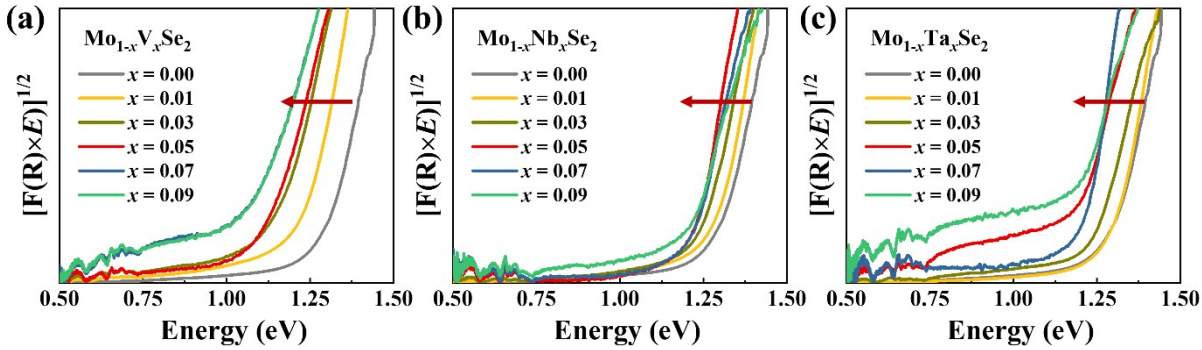

Fig. S4 Optical absorption spectra of $Mo_{1-x}M_xSe_2$ ($0 < x \leq 0.09$) compounds, where (a) M = V, (b) M = Nb, and (c) M = Ta. The optical absorption edge of the compounds shifts towards low energy with the increasing V/Nb/Ta content, and indicates a decreased band gap.

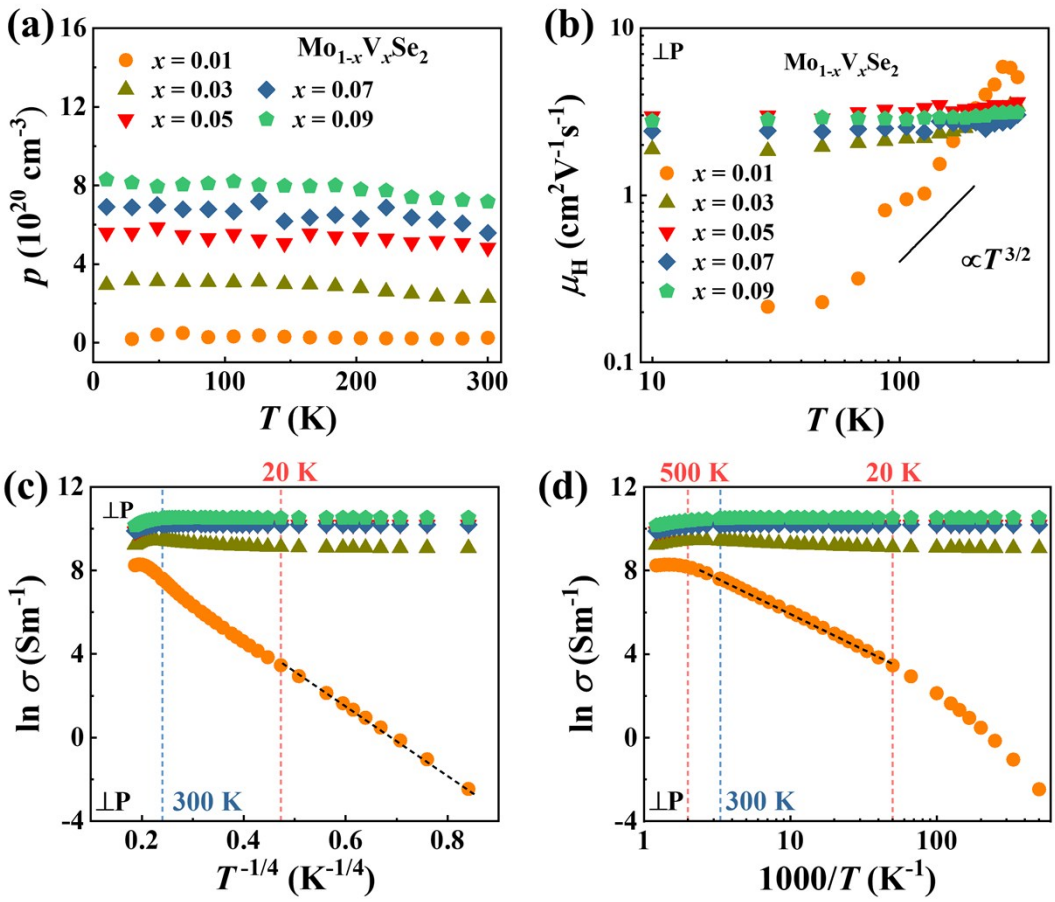

Fig. S5 (a) Temperature-dependent hole concentration and (b) the carrier mobility of $Mo_{1-x}V_xSe_2$ ($0 < x \leq 0.09$) compounds along ⊥P direction and within 10 – 300 K. (c) Temperature dependent electrical conductivity σ of $Mo_{1-x}V_xSe_2$ ($0 < x \leq 0.09$) along ⊥P direction in coordinates of $\ln\sigma = f(T^{-1/4})$, and (d) in $\ln\sigma = f(1000/T)$ in the range of 2 – 823 K.

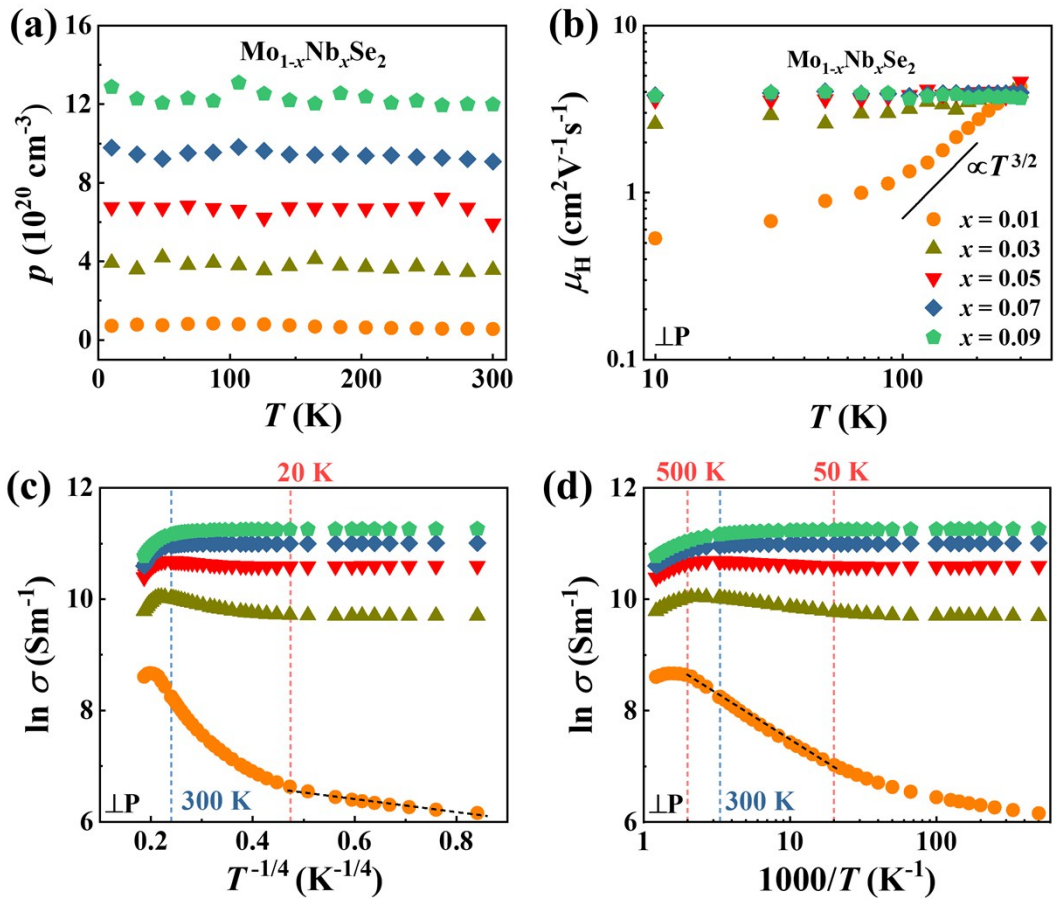

Fig. S6 (a)Temperature-dependent hole concentration and (b) the carrier mobility of $Mo_{1-x}Nb_xSe_2$ ($0 < x \leq 0.09$) compounds along ⊥P direction and within 10 – 300 K. (c) Temperature dependent electrical conductivity σ of $Mo_{1-x}Nb_xSe_2$ ($0 < x \leq 0.09$) along ⊥P direction in coordinates of $\ln\sigma = f(T^{-1/4})$, and (d) in $\ln\sigma = f(1000/T)$ in the range of 2 – 823 K.

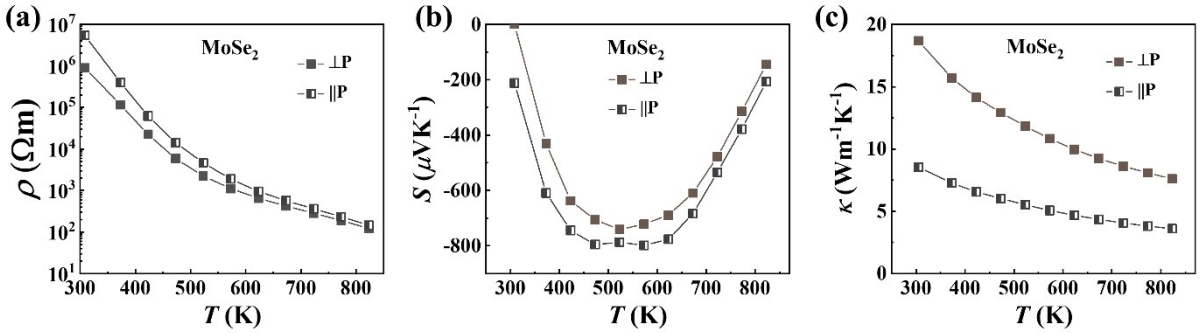

Fig. S7 Temperature dependence of (a) electrical resistivity, (b) the Seebeck coefficient, and (c) the thermal conductivity of the $MoSe_2$ compound measured along ⊥P and ||P directions. $MoSe_2$ has a layered structure with weak vdW bonds between the layers, resulting in distinctly different thermal transport properties of the bulk along the ⊥P direction and along the ||P direction.

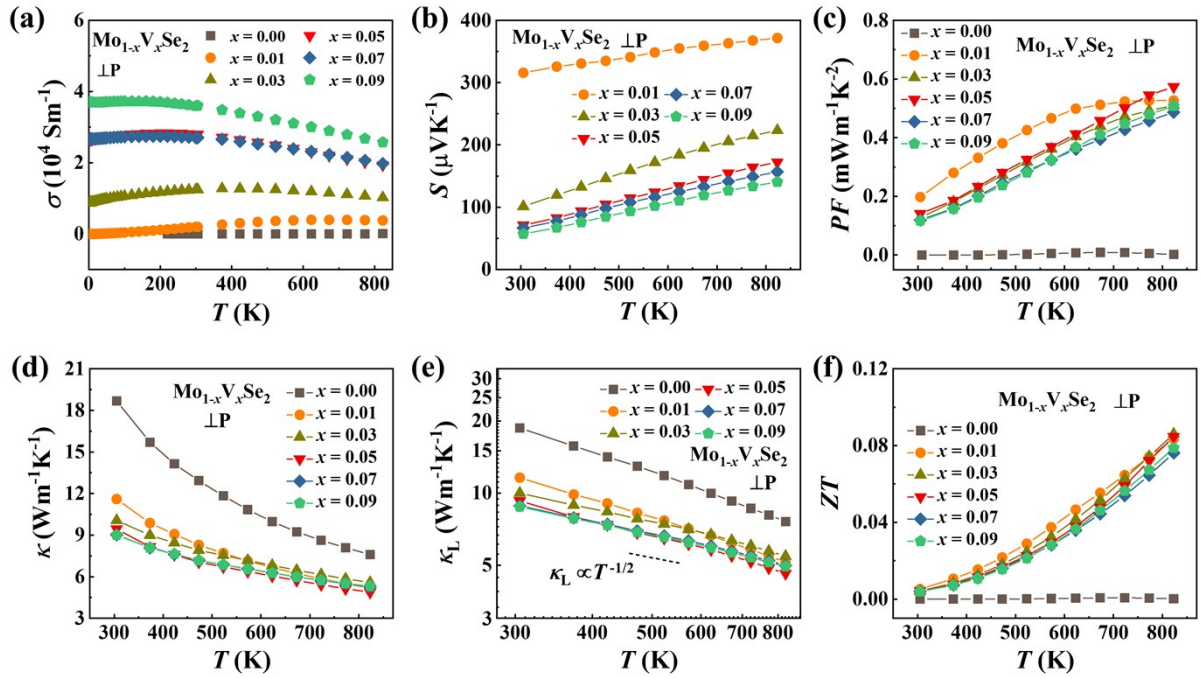

Fig. S8 Temperature dependence of (a) electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) thermal conductivity, (e) lattice thermal conductivity, (f) dimensionless figure of merit ZT of $Mo_{1-x}V_xSe_2$ ($0 < x \leq 0.09$) compounds measured along ⊥P direction.

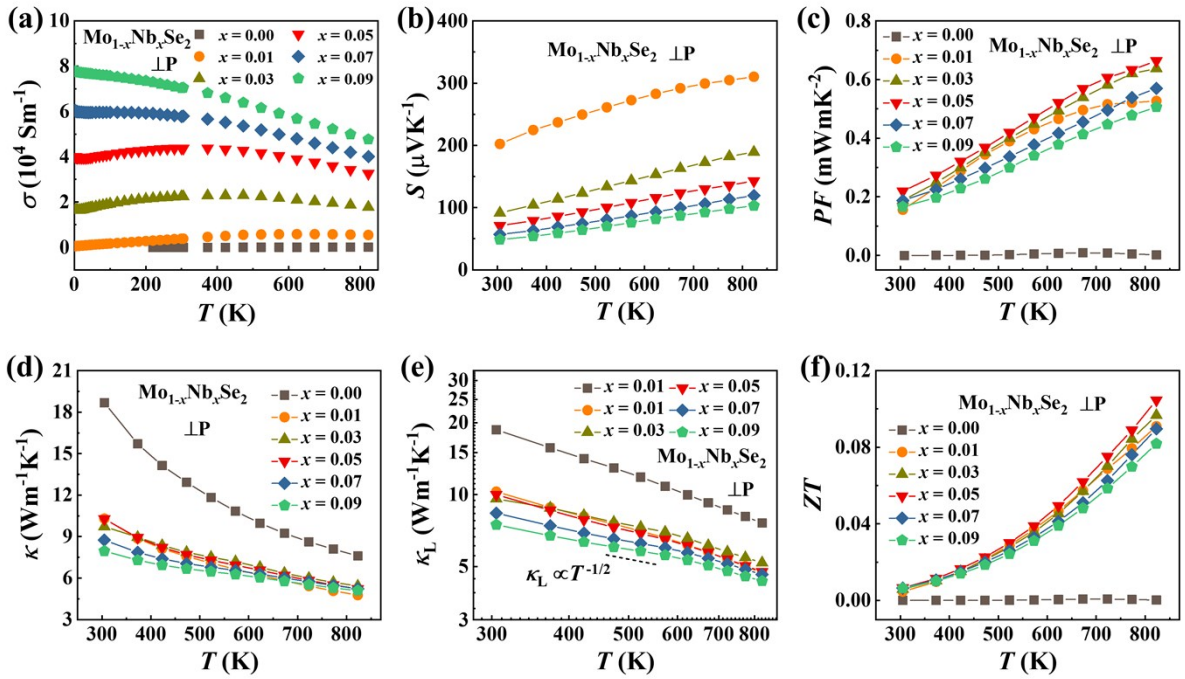

Fig. S9 Temperature dependence of (a) electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) thermal conductivity, (e) lattice thermal conductivity, (f) dimensionless figure of merit ZT of $Mo_{1-x}Nb_xSe_2$ ($0 < x \leq 0.09$) compounds measured along ⊥P direction.