Electronic Supplementary Information (ESI)

Large Nernst Power Factor over a Broad Temperature Range in Polycrystalline Weyl Semimetal NbP

Chenguang Fu,*‡^a Satya N. Guin,‡^a Sarah J. Watzman,^{a,b} Guowei Li, ^a Enke Liu,^a Nitesh Kumar,^a Vicky Süß,^a Walter Schnelle,^a Gudrun Auffermann,^a Chandra Shekhar,^a Yan Sun,^a Johannes Gooth,^a and Claudia Felser*^a

^aMax Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany ^bDepartment of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH 43210, USA

E-mail: Chenguang.Fu@cpfs.mpg.de, Claudia.Felser@cpfs.mpg.de [‡]These authors contributed equally.



Fig. S1 Powder XRD pattern for NbP with simulated pattern.

Table S1. Relative density of bulk NbP under different sintering temperatures.

| Bullz NhP somplo | Uniaxial pressure | Sintering temperature | Relative density | |
|------------------|-------------------|-----------------------|------------------|--|
| Buik Nor sample | (MPa) | (°C) | | |
| S1 | 80 | 800 | 59% | |
| S2 | 80 | 920 | 65% | |
| S3 | 80 | 970 | 71% | |
| S4 | 80 | 1150 | 91% | |
| S5 | 80 | 1200 | 91% | |



Fig. S2 SEM secondary electron image (a) and back scattered (BS-SEM) image (b) for polycrystalline NbP.

Table S2. Atomic percentage of NbP sample at 8 randomly selected positions detected by Energydispersive X-ray spectroscopy (EDX).

| element | Position 1 | Position 2 | Position 3 | Position 4 | Position 5 | Position 6 | Position 7 | Position 8 |
|---------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| Nb | 49.43% | 49.44% | 49.73% | 49.88% | 49.69% | 49.47% | 49.94% | 49.31% |
| Р | 50.57% | 50.56% | 50.27% | 50.12% | 50.31% | 50.53% | 50.06% | 50.69% |



Fig. S3 Schematically showing the as-sintered bulk sample. The thermal gradient (ΔT) and current (*I*) were applied along longer direction of the sample. The magnetic field ($B = \mu_0 H$) was applied parallel to the width of the sample during the transport measurement.

Definition of parameters

The Seebeck and Nernst effects are longitudinal and transverse thermoelectric responses, respectively. In order to make the description clear in the main text, here we first give a definition of all the transport parameters and their respective directions. The bulk sample of NbP after SPS is cylindrical. We define the height direction as the *z*-axis, while the plate face is the *xy*-plane, as shown in Figure S3. For a polycrystalline sample, there are should be no obvious differences in transport properties in-plane; thus, we consider the sample isotropic. Two bar-shaped samples are cut for transport measurements. We define the length direction as the *x*-axis while the width direction is the *y*-axis. The temperature gradient ΔT is applied along the *x*-axis while the magnetic field *B* is applied along the *z*-axis. The transport parameters are defined as shown in Table S3.

| Symbol | Transport parameter | Symbol | Transport parameter |
|------------------------------------|--|-------------------------------------|---|
| a _{xx} | Seebeck thermopower $(\mu V/K)$ | a _{xy} | Nernst thermopower ($\mu V/K$) |
| $\rho_{\rm xx}$ | Electrical resistivity (Ω cm) | $ ho_{\mathrm{xy}}$ | Hall resistivity (Ω cm) |
| $\sigma_{\rm xx}, \sigma_{\rm yy}$ | Electrical conductivity (Ω^{-1} cm ⁻¹) | $\sigma_{\rm xy}$ | Hall conductivity (Ω^{-1} cm ⁻¹) |
| K _{xx} | Thermal conductivity (W m ⁻¹ K ⁻¹) | | |
| PF = | Power factor (10^{-4} W m ⁻¹ K ⁻²) | $PF_{Nernst} =$ | Nernst power factor (10 ⁻⁴ W m ⁻¹ K ⁻²) |
| $\alpha_{xx}^2 \cdot \sigma_{xx}$ | | $\alpha_{xy}^{2} \cdot \sigma_{yy}$ | |
| zT | Thermoelectric figure of merit | zT _{Nernst} | Nernst figure of merit |

Table S3. Definition of the transport parameters.

The longitudinal and Hall conductivities are related to the resistivities via:

$$\sigma_{xx} = \frac{\rho_{xx}}{\rho_{xx}^2 + \rho_{xy}^2} \quad \text{and} \quad \sigma_{xy} = -\frac{\rho_{xy}}{\rho_{xx}^2 + \rho_{xy}^2} \tag{1}$$

The thermoelectric figure of merit $zT_{\rm S}$ is calculated according to the expression:

$$zT = \frac{\alpha_{xx}^2 \sigma_{xx}}{\kappa_{xx}} T$$
⁽²⁾

The Nernst figure of merit zT_{Nernst} is calculated using the formula:

$$zT_{Nernst} = \frac{\alpha_{xy}^2 \sigma_{yy}}{\kappa_{xx}} T$$
(3)



Fig. S4 Nernst coefficient versus temperature at low magnetic field ($\mu_0 H$) and high- $\mu_0 H$ region for polycrystalline NbP.



Fig. S5 Temperature dependent zT and zT_{Nernst} for polycrystalline NbP at different magnetic fields.