SUPPLEMENTARY INFORMATION FOR:

**Realizing *p*-type NbCoSn half-Heusler compounds with enhanced thermoelectric performance via Sc substitution**

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**Table S1** Physics parameters values: Debye temperature ***θ*D**, the sound velocity ***νs***, Grüneisen parameter ***γ***, deformation potential ***Edef***, density of state ***m*d\***, the longitudinal sound velocity ***νl*** and grain size ***d*** for transport properties calculation.

|  |  |  |
| --- | --- | --- |
| Parameters | Value  | References |
| *θ*D | 361 K | [1] |
| *νs* | 3141 m/s | [1] |
| *γ* | 1.2 | \* |
| *Edef* | 4.47 | [2] |
| *m*d\* | 3.4 | \*\* |
| *νl* | 4956 m/s | \* |
| *d* | 100-500 *μ*m | Figure S1 |

 \* fitting data \*\* calculated data

**Table S2** The average atomic mass of the crystal ***M*** and the average volume/atom ***Ω*** of Nb1-*z*Sc*z*CoSn.

|  |  |  |
| --- | --- | --- |
| Compositions  | *M* | *Ω* (10-30 m3/atom) |
| Nb0.99Sc0.01CoSn | 90.02 | 70.50 |
| Nb0.97Sc0.03CoSn | 89.70 | 70.52 |
| Nb0.96Sc0.04CoSn | 89.54 | 70.50 |
| Nb0.95Sc0.05CoSn | 89.38 | 70.60 |
| Nb0.94Sc0.06CoSn | 89.22 | 70.70 |
| Nb0.93Sc0.07CoSn | 89.06 | 70.70 |
| Nb0.90Sc0.10CoSn | 88.58 | 71.20 |



**Figure S1** Typical scanning electron microscopy image of Nb0.93Sc0.07CoSn.

**References**

[1] Ferluccio D A, Smith R I, Buckman J, et al. Impact of Nb vacancies and p-type doping of the NbCoSn-NbCoSb half-Heusler thermoelectrics. Phys Chem Chem Phys. 2018;20:3979-3987.

[2] Zhou J, Zhu H, Liu T-H, et al. Large thermoelectric power factor from crystal symmetry-protected non-bonding orbital in half-Heuslers. Nat Commun. 2018;9:1721.