Electronic Supplementary Material (ESI) for Dalton Transactions.

Enhancement of thermoelectric properties of Zintl phase $SrMg_2Bi_2$ by Na-doping

Fang Yu[a], Xiang Meng[b,*], Lu Li[b], and Cuilian Wen[c,**]

[a]Institute of Logistics Science and Engineering, Shanghai Maritime University, Shanghai 201306, China.

[b]School of Material Science and Engineering, Chongqing University of Arts and Sciences, Chongqing 402160, China

[c]College of Materials Science and Engineering, Fuzhou University, Xueyuan Road, Fuzhou 350108, China

*Email: xiang.meng@hotmail.com (X. Meng); clwen@fzu.edu.cn (C. Wen)

The single parabolic band (SPB) model:

The Seebeck coefficient:

$$S(\eta) = \frac{k_B}{e}\left[\frac{(r+5/2)F_{(r+3/2)}(\eta)}{(r+3/2)F_{(r+1/2)}(\eta)} - \eta\right]$$

The Hall carrier concentration:

$$n_H = \frac{1}{eR_H} = \frac{(2m^* k_B T)^{3/2}}{3\pi^2 h^3}\frac{(r+3/2)^2 F^2_{(r+1/2)}(\eta)}{(2r+3/2)F_{(2r+1/2)}(\eta)}$$

The Hall mobility:

$$\mu_H = \left[\frac{e\pi\hbar^4}{\sqrt{2}(k_B T)^{3/2}}\frac{C_1}{m^{*3/2}_b m^*_I E^2_{def}}\right]\frac{(2r+3/2)F_{(2r+1/2)}(\eta)}{\left(r+\frac{3}{2}\right)^2 F_{(r+1/2)}(\eta)}$$

Lorenz Factor:

$$L = \left(\frac{k_B}{e}\right)^2\left\{\frac{(r+7/2)F_{(r+5/2)}(\eta)}{(r+3/2)F_{(r+3/2)}(\eta)} - \left[\frac{(r+5/2)F_{(r+3/2)}(\eta)}{(r+3/2)F_{(r+1/2)}(\eta)}\right]^2\right\}$$

Where $F_j(\eta) = \int_0^\infty \frac{\xi^f d\xi}{1+exp(\xi-\eta)}$ is the Fermi integral, $m^* = \frac{h^2}{2k_B T}\left[\frac{n \times r_H}{4\pi F_{1/2}(\eta)}\right]^{2/3}$ is the density-of-states effective mass.

In the above equations, k_B is the Boltzmann constant, $\hbar$ is the reduced Plank constant, C_l is the elastic constant for longitudinal vibrations, E_{def} is the deformation potential coefficient characterizing the strength of carriers scattered by acoustic phonons, m_I^* is the inertial effective mass, m_b^* is the band effective mass and η is the reduced Fermi level. When charge carriers are scattered by the acoustic phonons, r=-1/2.

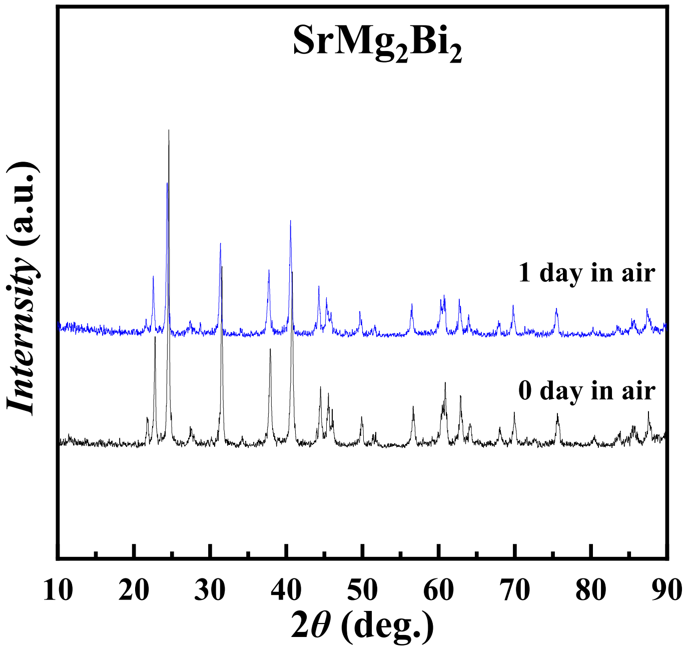

Figure S1 XRD patterns for $SrMg_2Bi_2$ kept in air for 0 and 1day.