

# Potential Thermoelectric Material $Tl_3XS_4$ ( $X =$ $V, Nb, Ta$ ) with Ultralow Lattice Thermal Conductivity

Xiefei Song <sup>\*a</sup>, Guangzhao Wang <sup>b</sup>, Wenzhong Li <sup>a</sup>, Siyu Gan <sup>d</sup>, Yan Cai <sup>a</sup>, Dianxu Ma <sup>a</sup>,  
Yuhui Luo <sup>a</sup>, Yao He <sup>\*c</sup> and Ning Wang <sup>\*d</sup>

<sup>a</sup> College of Physics and Information Engineering, Zhaotong University, Zhaotong 657000,  
Yunnan, China

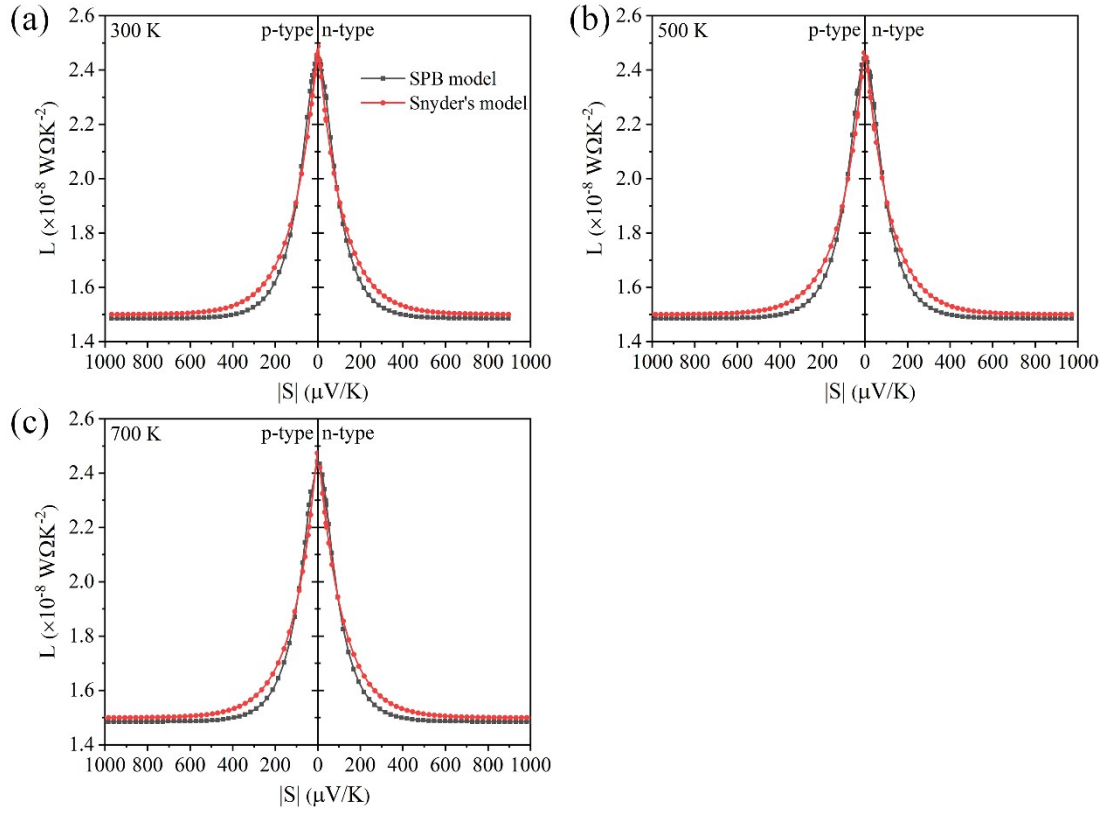
<sup>b</sup> Key Laboratory of Extraordinary Bond Engineering and Advanced Materials Technology of  
Chongqing, School of Electronic Information Engineering, Yangtze Normal University,  
Chongqing 408100, China

<sup>c</sup> Department of Physics, Yunnan University, Kunming 650091, China

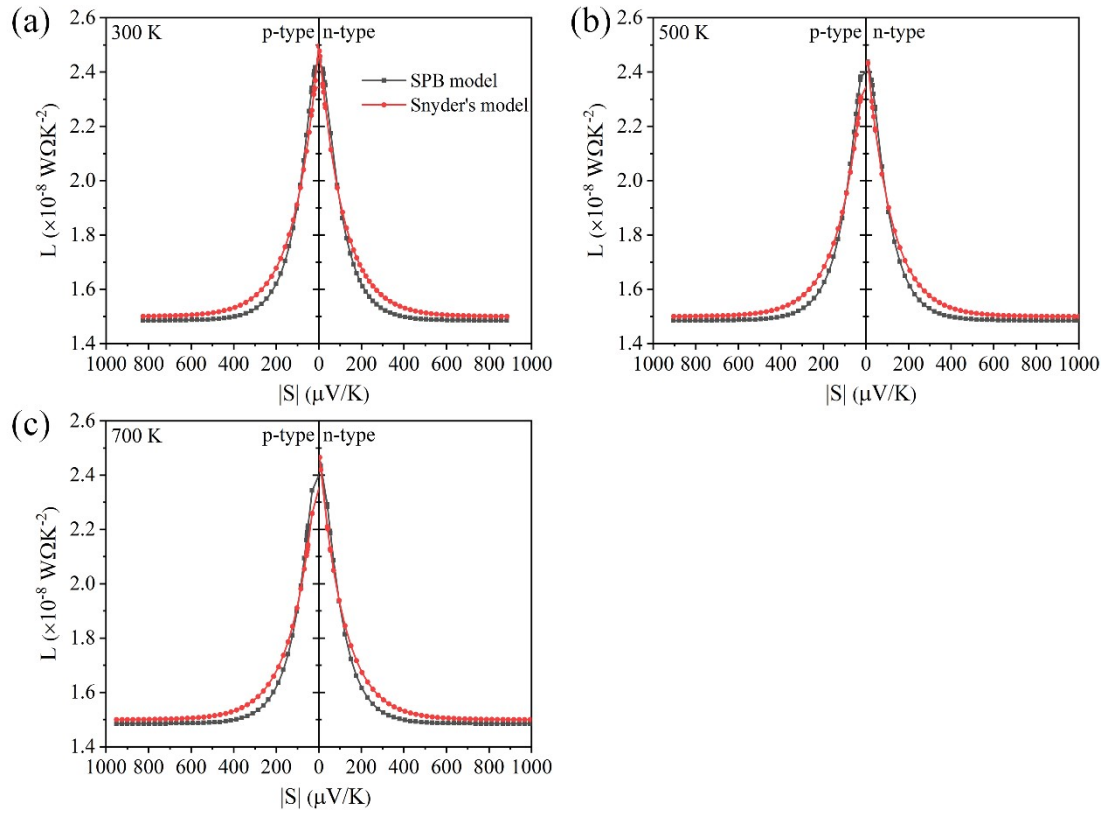
<sup>d</sup> School of Science, Key Laboratory of High Performance Scientific Computation, Xihua  
University, Chengdu 610039, Sichuan, China

\* Corresponding author.

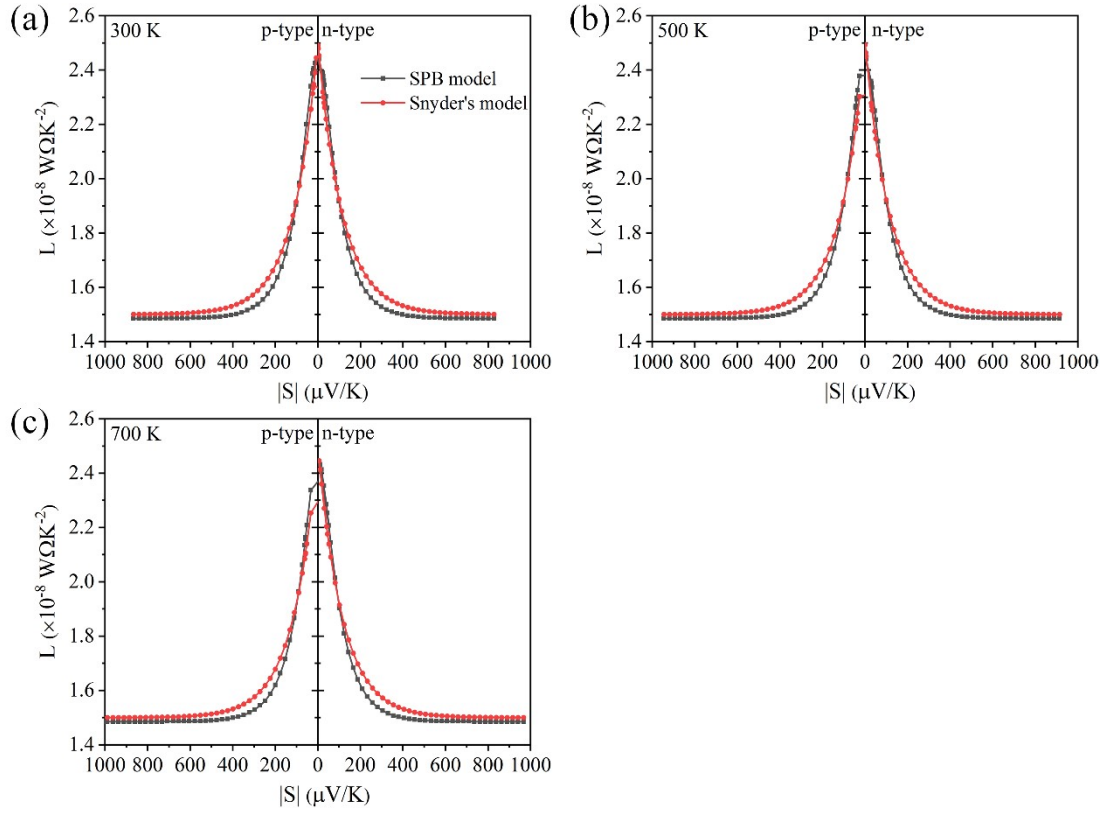
E-mail: xiefsong2023@163.com (Xiefei Song), yhe@ynu.edu.cn (Yao He),  
ningwang0213@163.com (Ning Wang)



**Figure. S1** The absolute Seebeck coefficient  $|S|$  dependent Lorenz number calculated by the SPB model and Snyder's model of  $\text{Tl}_3\text{VS}_4$  at 300 K (a), 500 K (b), and 700 K (c).



**Figure. S2** The absolute Seebeck coefficient  $|S|$  dependent Lorenz number calculated by the SPB model and Snyder's model of  $Tl_3NbS_4$  at 300 K (a), 500 K (b), and 700 K (c).



**Figure. S3** The absolute Seebeck coefficient  $|S|$  dependent Lorenz number calculated by the SPB model and Snyder's model of  $\text{Tl}_3\text{TaS}_4$  at 300 K (a), 500 K (b), and 700 K (c).