



Supporting Information

Biaxial Tensile Strain-Induced Enhancement of Thermoelectric Efficiency of α -Phase Se_2Te and SeTe_2 Monolayers

Shao-Bo Chen ^{1,2}, Gang Liu ³, Wan-Jun Yan ², Cui-E Hu ^{4,*}, Xiang-Rong Chen ^{1,*} and Hua-Yun Geng ⁵

¹¹ College of Physics, Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610064, China; shaobochoen@yeah.net

² College of Electronic and Information Engineering, Anshun University, Anshun 561000, China; yanwanjun7817@163.com

³ School of Physics and Engineering, Henan University of Science and Technology, Luoyang 471023, China; liugang8105@haust.edu.cn

⁴ College of Physics and Electronic Engineering, Chongqing Normal University, Chongqing 400047, China

⁵ National Key Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, CAEP, Mianyang 621900, China; s102genghy@caep.cn

* Correspondence: cuiehu@cqu.edu.cn (C.-E.H.); xrchen@scu.edu.cn (X.-R.C.)

Citation: Chen, S.-B.; Liu, G.; Yan, W.-J.; Hu, C.-E.; Chen, X.-R.; Geng, H.-Y. Biaxial Tensile Strain-Induced Enhancement of Thermoelectric Efficiency of α -Phase Se_2Te and SeTe_2 monolayers. *Nanomaterials* **2022**, *12*, 40. <https://doi.org/10.3390/nano12010040>

Academic Editor: Gyaneshwar P. Srivastava

Received: 4 November 2021

Accepted: 17 December 2021

Published: 23 December 2021

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).

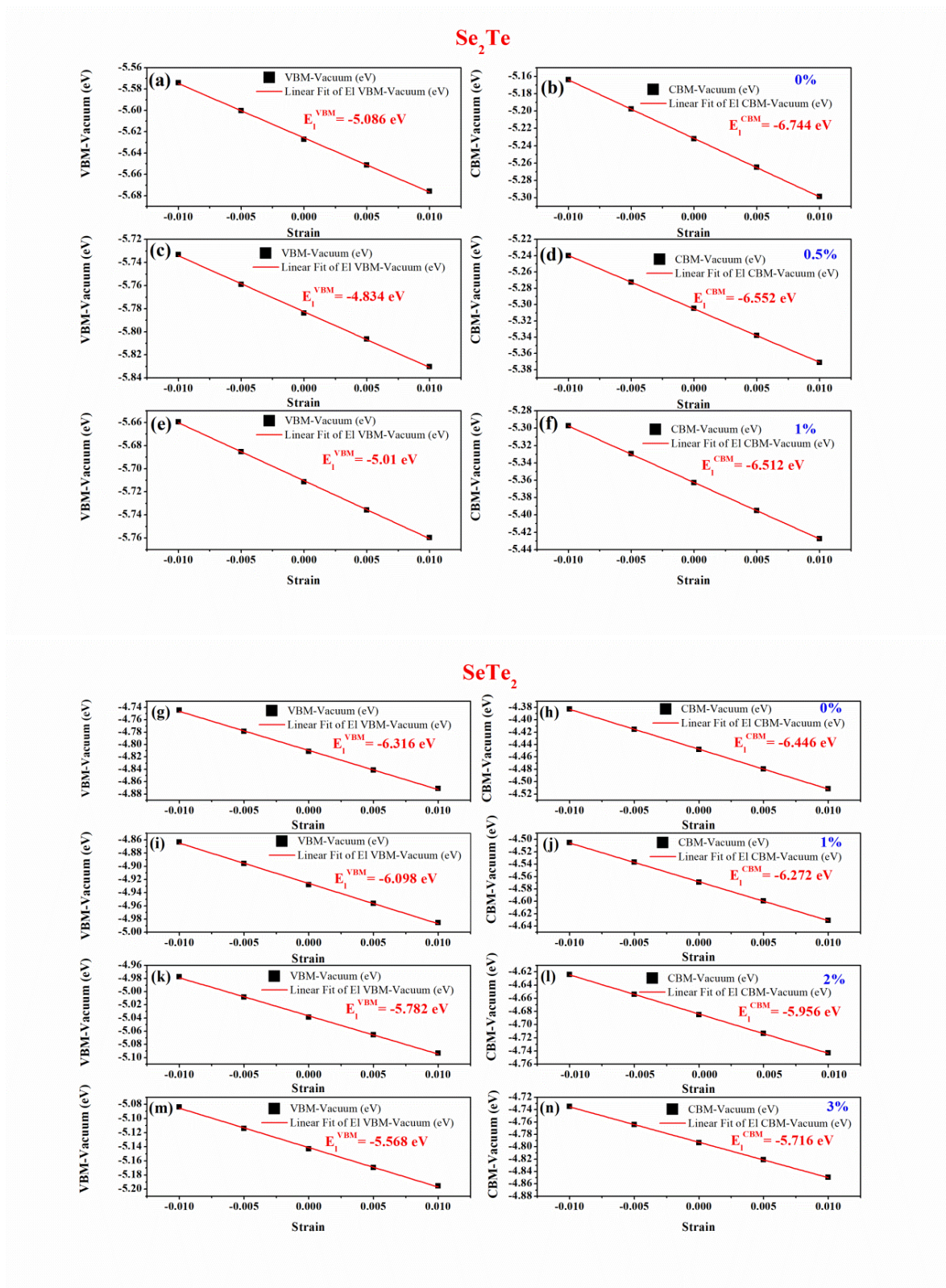


Figure S1. (Color online) The strain-dependent of deformation potential constants E_1 of α -phase (a-f) Se₂Te and (g-n) SeTe₂ monolayer based on PBE+SOC band structures, respectively. The red straight line is the linear fitting curve.

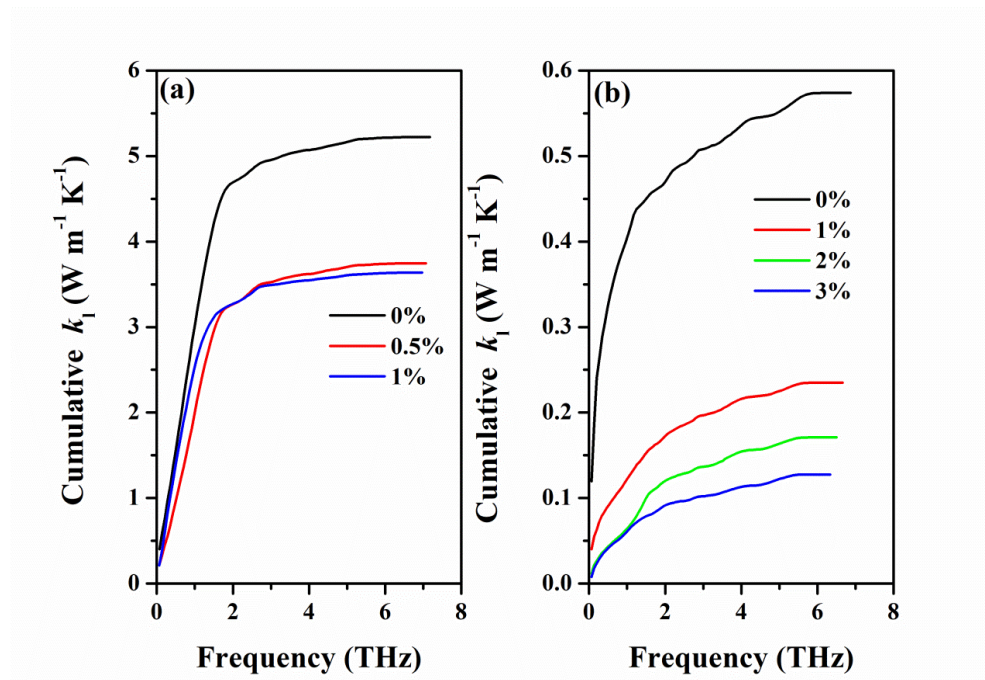


Figure S2. (Color online) The strain-dependent of cumulative k_l of (a) Se_2Te and (b) SeTe_2 monolayer at 300 K as a function of frequency, respectively.

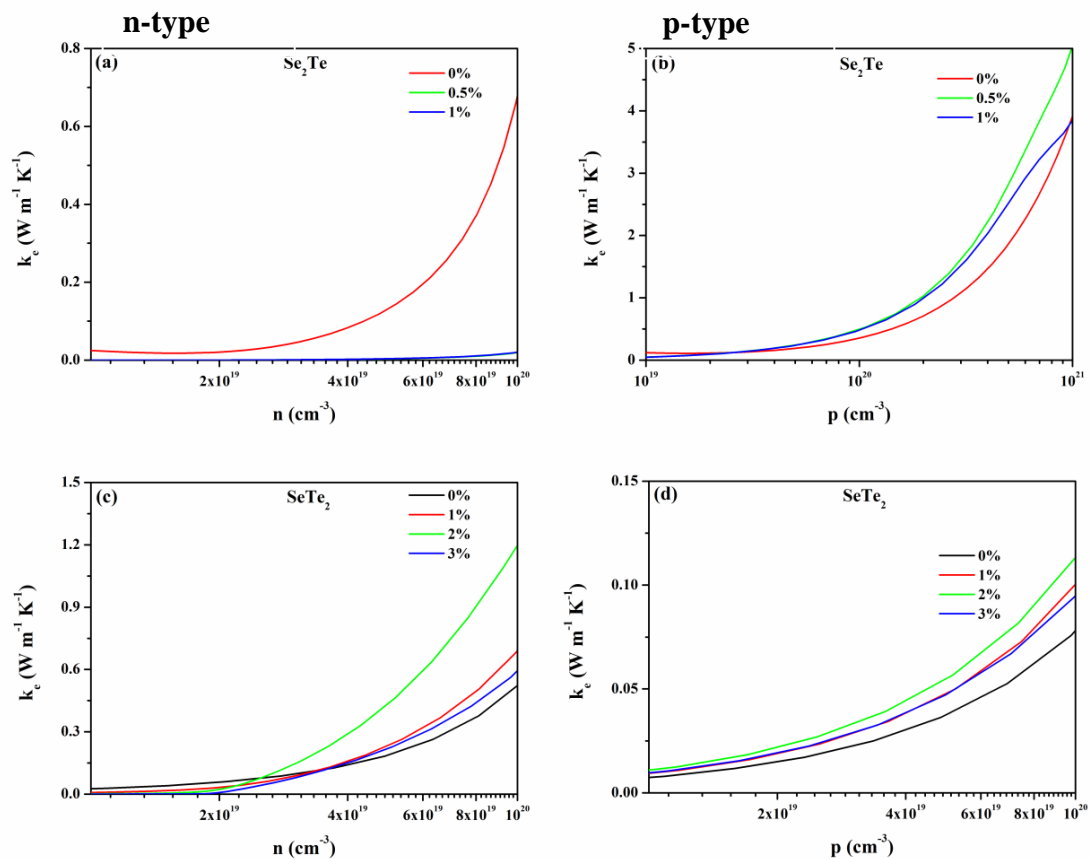


Figure S3. (Color online) The strain-dependent of electronic thermal conductivity k_e of (a, b) Se_2Te and (c, d) SeTe_2 monolayer at 300 K as a function of concentration for n-type and p-type doping, respectively.