

Supplementary Information

Oxidation-enhanced thermoelectric efficiency in a two-dimensional phosphorene oxide

Seungjun Lee¹, Jeong-Pil Song^{1,2}, Seung-Hun Kang^{1,3,*}, and Young-Kyun Kwon^{1,4,*}

¹Department of Physics, Kyung Hee University, Seoul, 02447, Korea

²Department of Physics, University of Arizona, Tucson, Arizona, 85721, United States of America

³Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, United States of America

⁴Department of Information Display and Research Institute for Basic Sciences, Kyung Hee University, Seoul, 02447, Korea

*Corresponding author: kangsh@ornl.gov, ykkwon@khu.ac.kr

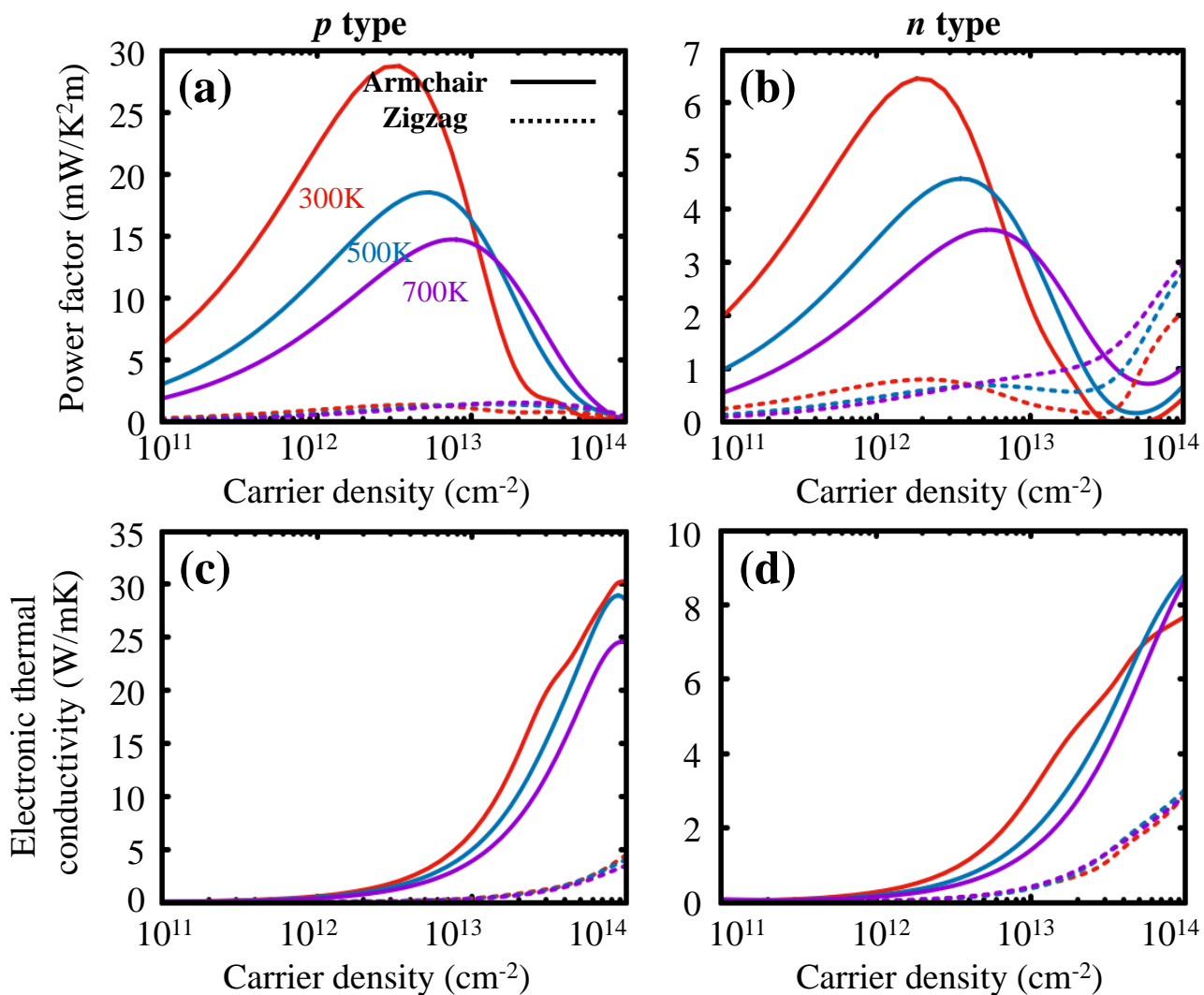


Figure S1. Power factors for (a) *p*-type and (b) *n*-type phosphorene and (c, d) their respective electronic thermal conductivities as a function of 2D carrier density. Solid and dashed lines denote these quantities computed along the armchair and zigzag transport directions at three different temperatures of 300, 500, and 700 K represented with the red, blue, and purple colors, respectively.

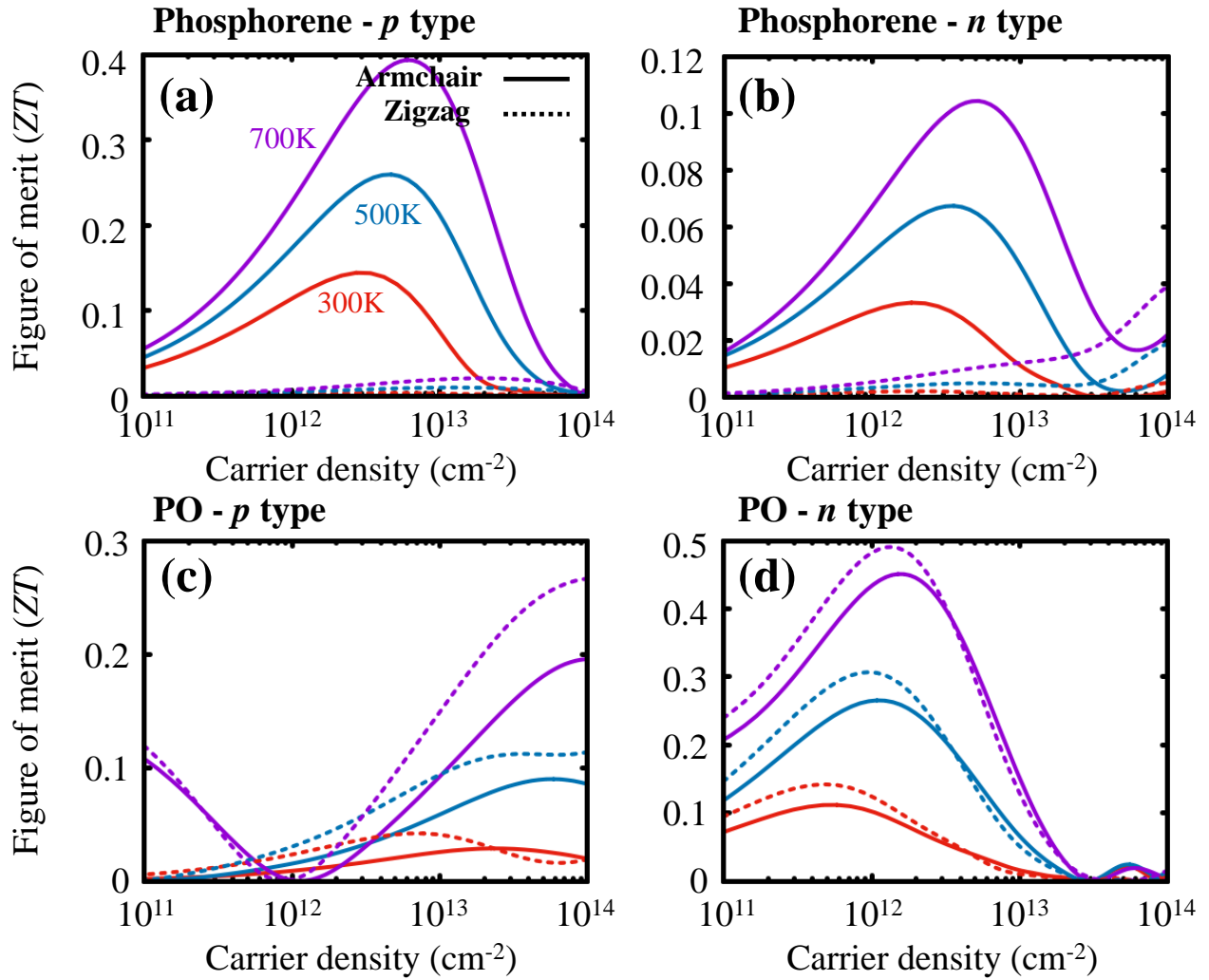


Figure S2. Thermoelectric figures of merit (ZT) of (a) p - and (b) n -doped phosphorene and (c, d) their PO counterparts as a function of 2D carrier density. Solid and dashed lines denote these quantities computed along the armchair and zigzag transport directions at three different temperatures of 300, 500, and 700 K represented with the red, blue, and purple colors, respectively.