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First-Principles Study on Thermoelectric Performance of Phosphorene and Phosphorene Oxide SEUNGJUN LEE, JEJUNE PARK, SEOUNG-HUN KANG, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul, 130-701, Korea — Using first-principles density functional theory, we studied thermoelectric properties of phosphorene and its oxidized structure called phosphorene oxide (PO). Using the identified stable configurations and electronic structrues of phosphorene and PO, we solved the Boltzmann transport equation to evaluate their electrical conductivity, Seebeck coefficient, and thermal conductivity contributed from both electrons and phonons. In order to correctly estimate the thermoelectric figure of merit or ZT values, it is indispensable to determine the relaxation time, which can be estimated by applying the deformation potential theory. We observe that the electrical conductivity of phosphorene is higher along the armchair direction than along the zigzag direction, while the thermal conductivity shows an opposite behavior. Because of such an orthogonal relation between the electrical and thermal conductivities, phosphorene exhibits quite a large ZT value along the armchair direction. It is, on the other hand, calculated that PO has electrical conductivity similar to phosphorene, however its thermal conductivity is significantly smaller than phosphorene, resulting in larger ZT values. we expect that PO can be utilized for a high performance thermoelectric application.

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