AB-INITIO STUDY OF THERMOELECTRIC PROPERTIES OF AN A,B_2,C_2 MATERIAL FOR WASTE HEAT RECOVERY FOR AN AUTOMOTIVE

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Abstract

Thermoelectric materials (TEM) convert temperature gradients directly into electricity and vice versa. Approximate 70% of the energy generated by the combustion of fuel in VVTI engine cannot be converted into mechanical energy, but disperses to the environment as waste heat. Reduction of energy consumption and curbing of CO_2 emissions of automotive becomes an important issue. The thermoelectric technology can convert heat into electric energy and improve the fuel efficiency of automotive. This paper studies the thermoelectric waste heat recovery system for automotive. TEM have received renewed interest for waste heat recovery and refrigeration applications. Their outstanding reliability due to the lack of moving parts makes them attractive candidates for a series of applications. However, today's thermoelectric devices are limited by their low efficiency and high costs. The density of states, band structure and figure of merit of AN A,B_2,C_2 material were calculated using computational methods. All calculations on the material were within the Density Functional Theory (DFT) framework and a plane wave basis set as implemented in the Quantum ESPRESSO and VASP codes. The Projector Augmented-Wave pseudopotentials was used to describe the core- valence electron interaction with PBE chosen for the exchange – correlation functional. The temperature dependent properties including thermoelectric transport properties were calculated using VASP code and analysed using the PHONOPY code. A comparison with previous DFT and Experimental studies were done. The figure of merit for the material was found to improve by 5%. The results obtained may lead to fabrication of devices in an automobile that convert waste heat energy to electricity. The A,B_2,C_2 thermoelectric devices obtained can be attached to the exhaust pipe to convert waste heat to electrical energy. The heat from cold side of thermoelectric devices is removed by liquid-cooling cold plate. A design of the heat exchanger of exhaust pipe to harvest heat of exhaust gas to thermoelectric modules effectively can be fabricated. The performance of thermoelectric waste heat recovery system with different designs is comprehensively studied.

Keywords: TEM, band gap, figure of merit.