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Mobility and thermoelectric properties of semiconducting diamanes C_2X (X=H, F, Cl)

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Abstract

In this paper, mobility and thermoelectric properties of diamanes C_2X (X = H, F, Cl) are studied using quantum espresso and Boltztrap computational package based on density functional theory. In all structures of C_2X (X = H, F, Cl), the mobility of holes is smaller than the mobility of the electrons, which is due to the shape of the band structure of each structure. Maximum of Seebeck coefficient is 2733, 2811, 2201 µV/K for n-type C_2H, $C_2F$and C_2Cl and it is -2767, -2696 and -2269 µV/K for p-type C_2H, $C_2F$and C_2Cl, respectively. In all structures, thermoelectric parameters such as electrical conductivity, electrical thermal conductivity and power factor are maximum in positive values of chemical potential. As a result, these materials can be more suitable thermoelectric materials with n-type doping. Also, all three structures have a maximum power factor in the temperature range of 200-500 Kelvin.

Keywords: mobility, thermoelectric, electrical conductivity, thermal conductivity, Seebeck coefficient, density functional theory

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