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

S Ahmadi Soltansaraie

Department of physics, Faculty of science, Imam Khomeini International University, Qazvin, Iran

E-mail: s.ahmadi@sci.ikiu.ac.ir

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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  $\mu V/K$  for n-type  $C_2H$ ,  $C_2F$  and  $C_2Cl$  and it is -2767, -2696 and -2269  $\mu V/K$  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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