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First-principles study of 2D electride : Gadolinium carbide
CHANDANI NANDADASA, SEONG-GON KIM, SUNGHO KIM, Mississippi State University, Starkville, MS39762, SUNG WNG KIM, sungkyunkwan university, Suwon, Korea — Electrides are an exclusive class of ionic compounds in which some electrons are occupying crystal voids instead of attaching to specific atoms or bonds. Using first-principles density functional theory calculations, we study structural, electronic and magnetic properties of Gd_2C. The theoretically predicted structure of Gd_2C is in good agreement with the available experimental data. Energy band diagram of Gd_2C shows that they are crossing the Fermi level. Projected electronic density of states plots indicate that the interstitial sites are the main contributor to the density of states at the Fermi level. Charge of individual atoms including interstitial site are obtained using Bader analysis. Magnetic properties of Gd_2C is determined from magnetization density plots. Work functions of Gd_2C are determined for (001) and (100) surfaces with the technique of macroscopic average of electrostatic potential with the Fermi energy of bulk.

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