

## عنوان مقاله:

The interface of FeCrP film with graphene-like BN: electronic, band alignment, and thermoelectric properties

## محل انتشار:

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## خلاصه مقاله:

Based on the Density Functional Theory (DFT) and Generalized Gradient Approximation (GGA), the structural, electronic, and band alignment properties of the interface of FeCrP film with graphene-like BN (g-BN) were studied. These properties have been investigated at three different distances between FeCrP film and g-BN. In all three mentioned distances, the ground state point and the bulk modulus show that these compounds have the necessary strength to form, and at the distance of  $2.7628 \text{ \AA}$ , the compound is more stable than the other two distances. At this interface, the bulk modulus is greater than its values for the pure FeCrP and also the g-BN compounds. In addition, at the FeCrP-BN interface, the emergence of a large magnetic moment of  $13.995 \mu_B$  is found. Based on the mBJ approximation, this interface has a half-metallic characteristic and in the minority spin, it has a direct bandgap of  $0.41 \text{ eV}$  spin flip. At this interface, the Schottky height was obtained to be about  $1.89 \text{ eV}$ . It is found that the BN electronic structure is n-type and the ECNLs appearing in this band alignment are close to the Fermi level as donor-like

## کلمات کلیدی:

FeCrP-BN interface, DFT, Electronic, Band alignment, Thermoelectric

## لینک ثابت مقاله در پایگاه سیویلیکا:

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