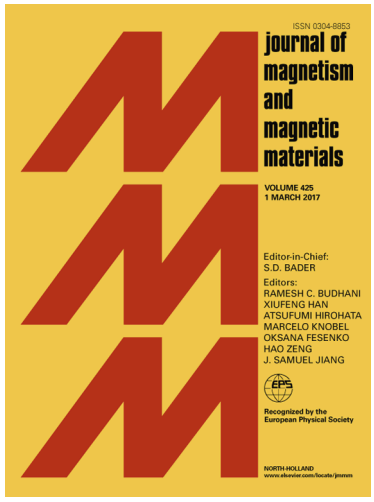

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Density functional theory study of tunable electronic and magnetic properties of monolayer BeO with intrinsic vacancy and transition metal substitutional doping

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Abstract

The anomalous electronic and magnetic properties of monolayer BeO with intrinsic vacancy and transition metal (TM) substitutional doping are investigated by means of extensive density functional theory calculations. Our calculations reveal that the Be vacancy (V_{Be}) can give rise to a stable ferromagnetism, while the O vacancy (V_O) does not show spin dependent electronic properties. More significantly, the monolayer BeO with V_{Be} becomes the magnetic semiconductor with a direct band gap (0.97 eV), whereas the band gap of the monolayer BeO with V_O drops to 3.56 eV, in comparison with the band gap of the pristine BeO (5.64 eV). It is found that the TM substituting Be atom (TM-BeO) is favorable and the ionic bonds are formed between TM and its neighboring O atoms. The electronic properties of the monolayer BeO are also considerably changed due to the induced impurity states. Only the Zn-BeO system preserves the nonmagnetic semiconductor characteristic, similar to the monolayer BeO. The Sc-, V-, Mn-, and Ni-BeO systems show dilute magnetic semiconductor (DMS) characters. More interestingly, the Ti-, Cr-, Fe-, Co- and Cu-BeO systems display half-metal characters.