

## Multiferroicity of magnesium hexaboride

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Hexaborides,  $MB_6$  ( $M=Ca, Sr, Ba$ ), have attracted considerable attention after the observation of a weak ferromagnetism not involving partially filled d or f orbitals. High melting point, chemical stability and high hardness are among other properties which raised the interest in these compounds. Although the above-mentioned systems were thoroughly investigated theoretically and experimentally, the properties of the lighter member of the family, namely  $MgB_6$ , are largely unknown so far. Our spin-polarized calculations, based on DFT at GGA level, predict multiferroicity in  $MgB_6$ , which is unique in this class of materials. In fact,  $MgB_6$  displays a weak magnetic moment associated with boron vacancies, similar to the ferromagnetism in the related  $CaB_6$  and  $SrB_6$ . In addition, a small Mg cation shift off the center of the simple cubic elementary unit cell breaks the central symmetry and yields the relatively large net electric dipole moment of 7.7 Debye per unit cell. Long range Coulombic interaction lowers the energy of the system further by arranging the dipoles in antiferroelectric order.