ELECTRONIC SPECTRA AND MAGNETIC PROPERTIES OF $R\mathbf{B}_6$, $R\mathbf{B}_{12}$ AND $R\mathbf{B}_2\mathbf{C}_2$ BORIDES

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9.7 cm

The electronic structures of $R\mathrm{B}_6$, $R\mathrm{B}_{12}$ and $R\mathrm{B}_2\mathrm{C}_2$ borides (where R is a rare-earth, alkaline-earth, or early transition metal atom) are studied *ab initio* by using the full-potential linear muffin-tin orbital method to shed light on the intriguing magnetic properties of these compounds. This includes the promising materials for spin electronics with reported high temperature ferromagnetism, namely, doped divalent hexaborides CaB_6, SrB_6, BaB_6, and the $\mathrm{CaB}_2\mathrm{C}_2$ compound, as well as Kondo semiconductors, SmB_6 and YbB_{12}. For CaB_6 and SrB_6 a semiconducting band structure has been obtained, in agreement with the recent experimental data, whereas a semimetallic ground state is expected for $\mathrm{CaB}_2\mathrm{C}_2$ and doped hexaborides. For $\mathrm{CaB}_2\mathrm{C}_2$ and the semimetallic $\mathrm{Ba}_{1-x}\mathrm{La}_x\mathrm{B}_6$ alloys we have performed spin-polarized calculations in an external field to evaluate the induced spin and orbital magnetic moments. The calculations indicate a possibility of the field-induced weak ferromagnetic phase in $\mathrm{CaB}_2\mathrm{C}_2$ and the La doped hexaborides. The LSDA and GGA calculations for different spin configurations of YbB_{12} point to a predominantly antiferromagnetic coupling between Yb^{+3} ions. For SmB_6 and YbB_{12} our LSDA, GGA, and LSDA+U calculations have not revealed the hybridization gap for configurations with trivalent Sm^{+3} and Yb^{+3}.

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