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Ground and excited state properties of CaB_6 determined byLDA and screened–exchange LDA investigations[1] Y.C. HSUE, J.E. MEDVEDEVA, A.J. FREEMAN, Northwestern Univ. — CaB_6 has recently attracted great interest because it exhibits weak high-temperature ferromagnetism when lightly doped by La and could possibly be useful in room temperature spintronic devices. In pure CaB_6, its semiconductor nature has now been established experimentally[2]. Questions about its theoretical description are centered about the fact that first principles LDA calculations underestimate band gaps and in CaB_6 results in a semi-metal with a 0.3 eV overlap at the X point. Here we use the full-potential linearized augmented plane wave method (FLAPW)[3] within both the LDA and the screened–exchange LDA (sX–LDA) to determine the ground and excited state properties of CaB_6. First, we did the geometry optimization with LDA and used this optimized structure in sX–LDA calculations. We find that CaB_6 is a semiconductor with a gap of 0.68 eV at X in agreement with the recent experimental results. We also calculated the optical properties with spin–orbit coupling and full matrix elements. Finally, results of similar calculations for Eu and La doped CaB_6 will be reported.

[1]Supported by Grant DARPA
[2]B.K. Cho, et.al., PRB 69, 113202 (2004) and references therein.
[3]Wimmer, Krakauer, Weinert and Freeman, PRB 24, 864(1981)

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