Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principles study on the surface half-metallicity of CaC in the zinc-blende structure[1] KAILUN YAO, GUOYING GAO, ZULI LIU, Huazhong University of Science and Technology — We investigate the electronic structure and the surface half-metallicity of CaC in the zinc-blende structure by using the first-principles full-potential linearized augmented plane-wave (FPLAPW) method. It is found that the (1 1 0) surface preserves the half-metallic character of the bulk, while in the case of the (0 0 1) surfaces including the Ca-terminated and C-terminated surfaces the surface states destroy the half-metallicity.

[1]This work was supported by the National Natural Science Foundation of China under Grant Nos. 10574047,10574048 and 20490210. It was also supported by National 973 project under grant No. 2006CB921600.

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Date submitted: 16 Nov 2007 Electronic form version 1.4