First-principles study on the surface half-metallicity of CaC in the zinc-blende structure 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.

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