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**Ab initio study of $d^{\bigcirc}$ magnetism in CaC** HADI AKBARZADEH, ZAHRA NOURBAKHSH, S. JAVAD HASHEMIFAR, Isfahan University of Technology — The half-metallic ferromagnetism in $d^0$ ionic compounds has attracted considerable attention in the spintronics community [Phys. Rev. B 73 024404, 2006]. In this work we employ density functional theory to study electronic, magnetic, and mechanical properties of the high ionic CaC compound in the Zinc Blend (ZB), Rock Salt (RS), $B_2$, Wurtzite (WZ), NiAs, and tetragonal structures.The observed ferromagnetic equilibrium state in the RS, NiAs, WZ, tetragonal and ZB structures is attributed to the partially filled sharp p band of carbon around the Fermi level. Half-metallicity has been found in the equilibrium ZB and expanded WZ structures with a magnetic moment of 2 $\mu_B$/formula units. Comparing the Gibbs free energy of various structures indicates favorability of the half metallic phases in negative pressures. Topological analysis of the electronic charge density reveals topological character of the paramagnetic-ferromagnetic phase transition of the revised NiAs and $B_2$ structures as well as the geometrical character of the magnetic phase transitions of the RS and ZB structures.

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