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NOVEL PREDICTION USING TB-mBJ OF ELECTRONIC PROPERTIES, MAGNETIC EXCHANGE COUPLINGS, AND HALF-METALLICITY IN CrCaSe MATERIALS †

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In this study, we have performed investigations on the structural stability, electronic band structures, magnetic exchange couplings, and half-metallic performance of $Cr_xCa_{1-x}Se$ materials using computational methods of density functional theory via GGA-WC, GGA-PBE and, TB-mBJ exchange-correlation potentials. The $Cr_xCa_{1-x}Se$ compounds are thermodynamically stable and synthesizable owing to their negative formation energies. The structural parameters of $Cr_xCa_{1-x}Se$ with GGA-WC and GGA-PBE approximations appear to be in excellent concordance compared to the experimental data and recent theoretical calculations. According to GGA-PBE and TB-mBJ calculations, the $Cr_xCa_{1-x}Se$ compounds revealed integral magnetic moments and a half-metallic behavior with better half-metallic gaps, and spin-polarization of 100%. The $Cr_xCa_{1-x}Se$ alloys appear to be better materials for use in spintronic devices.

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