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First-principles investigation of the effect of pressure on $CaFe_2As_2$ and Pr-doped $Ca_{1-x}Pr_xFe_2As_2$[1] TANJU GUREL, Department of Physics, Namik Kemal University, Tekirdag, TR-59030, Turkey, A. V. LUKOYANOV, Institute of Metal Physics, Ural Branch of Russian Academy of Sciences, 620990 Yekaterinburg, Russia and Ural Federal University, 620002 Yekaterinburg, ESRA ERTURK, Department of Physics, Namik Kemal University, Tekirdag, TR-59030, Turkey, GUVEN AKCAY, RESUL ERYIGIT, Department of Physics, Abant Izzet Baysal University, Bolu 14280, Turkey, V. I. ANISIMOV, Institute of Metal Physics, Ural Branch of Russian Academy of Sciences, 620990 Yekaterinburg, Russia and Ural Federal University, 620002 Yekaterinburg — In a recent study (arXiv:1310.3842), superconductivity has been observed at critical temperature 51 K under pressure 1.9 GPa for rare-earth doped $Ca_{0.86}Pr_{0.14}Fe_2As_2$ which is the highest T_c reported in the class of 1-2-2 iron-based superconductors. Motivated by this, we present density functional theory calculations on iron-based pnictide undoped $CaFe_2As_2$ and Pr-doped $Ca_{1-x}Pr_xFe_2As_2$ (x=0.25 and 0.125). The calculations have been carried out using plane-waves and pseudopotential approach within generalized gradient approximation (GGA) and also within GGA+U in order to investigate the influence of correlation effects. The effect of pressure on crystal structure, magnetic order, and electronic structure are investigated for both undoped and Pr-doped structures for comparison and discussed with experimental findings.

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