Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First principles investigation of Sr and P doping of $CaFe_2As_2$
HARALD O. JESCHKE, MILAN TOMIC, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — The doping-temperature-pressure phase diagrams of the 122 family of superconductors have been discussed intensively due to electronic nematicity above the structural and superconducting transition and the complex coupling between electronic and lattice degrees of freedom. We employ density functional theory to determine the structure of supercells of $Ca_{1-x}Sr_xFe_2As_2$ and $CaFe_2(As_{1-x}P_x)_2$. We then predict structural transitions of the doped compounds under pressure and compare to the parent compound. We carefully analyze the changes in the electronic structure caused by doping and stress.

Harald O. Jeschke
Institut für Theoretische Physik, Goethe-Universität Frankfurt,
Max-von-Laue-Str. 1, 60438 Frankfurt, Germany

Date submitted: 27 Nov 2012 Electronic form version 1.4