Abstract Submitted
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**Emergence of complex magnetism in three dimensional, yet quasi-layered, iron pnictides: $CaFe_4As_3$**[1] ARTHUR J. FREEMAN, GIANCARLO TRIMARCHI, MERCOURI KANATZIDIS, Northwestern U., ILIYA TODOROV, DUCK-YOUNG CHUNG, Materials Science Division, ANL, Argonne IL 60439 — The class of iron pnictides has been the focus of much attention for the discovery of superconductivity in the layered compounds LaOFeAs, $CaFe_2As_2$, and related ones; the phase diagrams of these pnictides remain still largely unexplored. Here, we report on the electronic and magnetic structure of the recently synthesized $CaFe_4As_3$ compound. This material, as opposed to the layered $CaFe_2As_2$, shows FeAs slabs parallel to the *b*-direction and approximately perpendicular to each other, defining tunnels filled by the Ca atoms. No sign of superconductivity was found in this compound. Instead, the system shows a complex ferromagnetic state at low temperature. DFT calculations performed on the refined crystal structure using the highly precise FLAPW method[2] show a pronounced stabilization for the ferromagnetic state which is characterized by four distinct Fe sites with magnetic moments of between 1 $\mu_B$ and 2 $\mu_B$. The influence of the local topology of the crystal structure on the the electronic and magnetic state is analyzed.

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[2]Wimmer, Krakauer, Weinert, and Freeman, PRB, **24**, 864 (1981)

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