

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Itinerant Nature of Magnetism in Iron Pnictides: A first principles study¹ YU-ZHONG ZHANG, INGO OPAHLE, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Unversitaet Frankfurt — The magnetic properties of LaFePnO , BaFe_2Pn_2 and LiFePn ($Pn = \text{As, Sb}$) are investigated by using *ab initio* molecular dynamics based on an all-electron projector-augmented wave basis. We find that stripe-type antiferromagnetic orderings are always enhanced when As is substituted by Sb. Our calculated Pauli susceptibility strongly points towards an itinerant picture of magnetism. Furthermore, we study the lattice properties of LaFePnO ($Pn=\text{P, As, Sb, Bi}$) as well as ScFePO , ScFeAsO and YFePO and argue that LaFeSbO would be a candidate for a superconductor with highest transition temperature among the investigated compounds.

¹This work was supported by the Deutsche Forschungsgemeinschaft through the TRR/SFB 49 and Emmy Noether programs.

Harald O. Jeschke
Institut fuer Theoretische Physik, Unversitaet Frankfurt

Date submitted: 06 Jan 2010

Electronic form version 1.4