**First Principles Investigations on a New 1111-type Fe-based Superconductor: ThFeAsN**

Smritijit Sen[1] and Guang-Yu Guo[1,2]

[1]*Department of Physics and Center for Theoretical Physics, National Taiwan University, Taipei 10617, Taiwan*

[2] *Physics Division, National Center for Theoretical Sciences, Hsinchu 30013, Taiwan*

Recent discovery of superconductivity at 30K in stoichiometric ThFeAsN compound [1], in absence of spin density wave order [2] stipulate a possibility of non-magnetic origin of high temperature superconductivity. In contrary to the experimental results, first principles calculation within GGA predicts a stripe antiferromagnetic ground state in this system [3]. In order to explore the emergence of superconductivity in ThFeAsN, we perform electronic structure calculations within density functional theory (DFT). Our first principles electronic structure calculations reveal the semi metallic behavior of ThFeAsN, which resembles with that of the LaFeAsO and most of the other Fe-based superconductors. Fig. 1 depicts our calculated orbital projected band structure of ThFeAsN in non-magnetic state. The dominance of Fe $d_{yz}$, $d_{xz}$ and $d_{xy}$ orbitals at the Fermi level is in well agreement with that of the previous experimental as well as theoretical results [1,4].

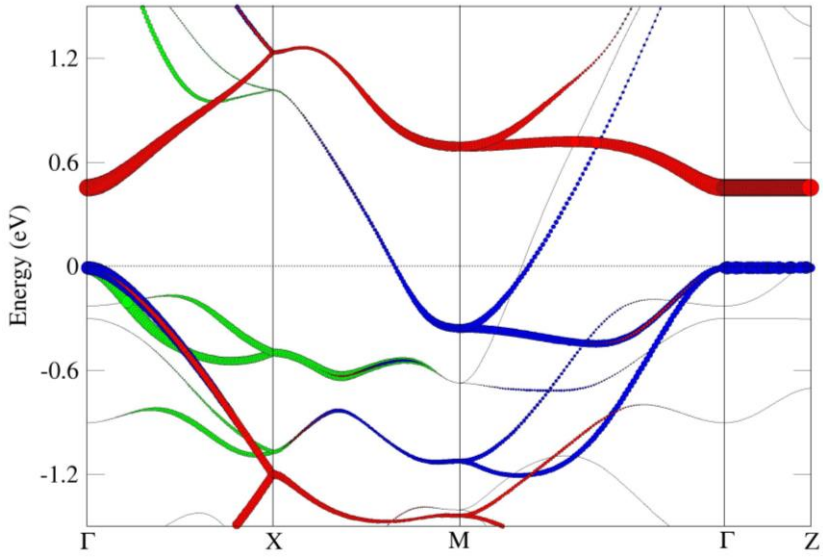


**Fig. 1:** *Calculated orbital projected [Fe- $d_{yz}$ (green), $d_{xz}$ (blue), $d_{xy}$ (red)] band structure of ThFeAsN with GGA optimized structure in non-magnetic state.*

Moreover, the role of electron-phonon coupling to superconductivity in this system is still not known [5]. In this work we present the electronic structures of ThFeAsN and the role of phonon in the mechanism of superconductivity in this system.

**References**

[1]. C. Wang *et al.*, J. Am. Chem. Soc. **138**, 2170 (2016).
[2]. M. A. Albedah *et al.*, J Alloys Compd. **695**, 1128 (2017)
[3]. G. Wang and X. Shi, Europhys. Lett. **113**, 67006 (2016).
[4]. D. J. Singh, J Alloys Compd. **687**, 786 (2016).