Abstract Submitted for the MAR15 Meeting of The American Physical Society

Carrier Mediated Ferromagnetism in Fe-doped SrTiO₃¹ CHUN-LAN MA, School of Mathematics and Physics, Suzhou University of Science and Technology, Suzhou 215009, China, ROCIO CONTRERAS-GUERRERO, RAVI DROOPAD, Ingram School of Engineering, Texas State University, San Marcos, TX 78666, USA, BYOUNGHAK LEE, Department of Physics, Texas State University, San Marcos, TX, 78666, USA — The discovery of III-V dilute magnetic semiconductors (DMSs) and the subsequent unsuccessful search for room temperature ferromagnetism in DMSs have motivated researches on alternate dilute magnetic systems. Recent progresses in thin flim growth techniques of perovskite oxides suggest that dilute magnetic oxides (DMOs) can be viable candidates to improve the magnetic properties of DMSs. In this talk we present an ab initio study of Fedoped SrTiO₃. We find that a ferromagnetic ordering among localized Fe t_{2g} spins is mediated by itinerant Fe e_g electrons. The exchange interaction between t_{2g} and e_q electrons depends on crystal field splitting, on-site electron-electron interaction, and the relative energy of Fe d-ortbitals to oxygen p-orbitals. The exchange coupling and the majority-minority spin splitting decrease with decreasing carrier concentration, confirming that itinerant carriers mediate the ferromagnetism.

¹C. Ma is supported by NSF of China (Grant Nos. 11247023 and 11304218), Jiangsu Qing Lan Project, and Jiangsu Overseas Research & Training Program. R.C.-G, R.D., and B.L. are supported by AFOSR, award number FA9550-10-1-0133.

Chun-Lan Ma School of Mathematics and Physics, Suzhou University of Science and Technology, Suzhou 215009, China

Electronic form version 1.4

Date submitted: 15 Nov 2014