

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Observation of room-temperature ferromagnetism in Cu:ZnO films part II; a theoretical study T. BERLIJN, W. KU, Brookhaven National Laboratory, T.S. HERNG, D.-C. QI, J.B. YI, K.S. YANG, National University of Singapore, Y. DAI, Shangdong University, Y.P. FENG, I. SANTOSO, National University of Singapore, C. SANCHEZ-HANKE, Brookhaven National Laboratory, X.Y. GAO, A.T.S. WEE, J. DING, A. RUSYDI, National University of Singapore — To better understand the observation of room-temperature ferromagnetic ordering in O-deficient Cu:ZnO films [1], we calculated the configuration-averaged spectral function $\langle A(k, \omega) \rangle$ of ZnO with 2% Cu impurities and 1% O vacancies within the “LDA+U” approximation, solving the Hamiltonian only within the low energy Hilbert space, defined via the first-principles Wannier functions [2]. Based on these first principles results we proposed a microscopic “indirect double-exchange” model for the FM in Cu:ZnO that explains our main experimental findings.

[1] T.S. Herng et al, Phys. Rev. Lett. **105**, 207201 (2010)

[2] T. Berlijn et al, arXiv:1004.1156 (2010)

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Date submitted: 29 Dec 2010

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