Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Occupied and Unoccupied Electronic Structure of Na doped MoS_2(0001) T. KOMESU, University of Nebraska, Lincoln, D. LE, University of Central Florida, X. ZHANG, University of Nebraska, Lincoln, Q. MA, University of California - Riverside, E. F. SCHWIER, Y. KOJIMA, M. ZHENG, H. IWASAWA, K. SHIMADA, M. TANIGUCHI, Hiroshima University, Japan, L. BARTELS, University of California - Riverside, T. S. RAHMAN, University of Central Florida, P. A. DOWBEN, University of Nebraska, Lincoln — The influence of sodium on the band structure of MoS_2(0001) and the comparison of the experimental band dispersion with density functional theory (DFT) shows excellent agreement for the occupied states (angle-resolved photoemission), and qualitative agreement for the unoccupied states (inverse photoemission spectroscopy). We will show that Na-adsorption leads to charge transfer to the MoS_2 surface causing an effect similar to n-type doping of a semiconductor. Moreover, results of our simulations and measurements clearly indicate that the MoS_2 occupied valence band structure shifts rigidly to greater binding with little change in the occupied state dispersion and that the unoccupied states shift downward, approaching the Fermi level, yet the amount of the shift for the unoccupied states is greater than that of the occupied states, effectively causing a narrowing of the bandgap. At higher Na coverages MoS_2 surafce becomes metallic. Details of electronic band structure of Na/MoS_2(0001) will be discussed in light of the role of the frontier orbitals in facilitating chemical reactivity of the system.

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Date submitted: 14 Nov 2014 Electronic form version 1.4