Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles study on the specific heat of optimally hole-doped BaFe2As2 compound HYUNGJU OH, SINISA COH, MARVIN L. COHEN, UC Berkeley, Lawrence Berkeley National Laboratory — We present density functional calculation of optimally K-doped BaFe2As2, including a modification of the GGA potential by adding a repulsive term (GGA+A). We tune the additional repulsive term until the occupied bandwidth of the M-point electron pocket agrees with experimental data. The calculated Sommerfeld coefficient and electron-phonon coupling constant yield a theoretical specific heat coefficient comparable to the experimental one. In addition, overall band structure and Fermi surface topology are improved with respect to the experiment. This work was supported by NSF Grant No. DMR10-1006184 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the DOE at Lawrence Berkeley National Laboratory's NERSC facility.

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Date submitted: 14 Nov 2014 Electronic form version 1.4