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Systematic study of the electronic structure of a doped Mott insulator P GANESH, J BALACHANDRAN, Oak Ridge National Laboratory, Y LUO, H SHIN, A BENALI, Argonne National Laboratory, P.R.C KENT, Oak Ridge National Laboratory, O HEINONEN, Argonne National Laboratory — Controlled manipulation of electronic properties of Mott insulators through doping is an important step towards realizing Mottronics. However, describing the electronic-structure of correlated electronic materials, such as doped Mott insulators, is challenging using conventional density functional theory (DFT) methods. A wide range of methods to correct for this deficiency in DFT has been recently proposed, such as SIC-DFT, DFT+U, hybrid-DFT etc. In this talk we will explore the sensitivity of these different methods, in describing the electronic-structure of K-doped NiO, and compare our predictions from these methods with those obtained from a more accurate many-body method, such as quantum monte-carlo (QMC), which accurately describes such correlated electron systems. We will address questions such as: Where are the holes located in K-doped NiO? How localized are they? How does the localization depend on the doping concentration, and affect the conductivity of the material? We will also contrast our results to Li-doped NiO, which has been experimentally studied before. Answers to these questions have serious ramifications to our ability to describe electronic phase transitions in doped solids where strong electron correlations dictate the underlying physics of the material. * This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Computational Materials Sciences Program.

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