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Quantum Monte Carlo study of a K-doped NiO Mott insulator<sup>1</sup> ANOUAR BENALI, HYEONDEOK SHIN, YE LUO, Argonne National Laboratory, JARON KROGEL, PANCHAPAKESAN GANESH, JANAKIRAMAN BALACHANDRAN, PAUL KENT, Oak Ridge National Laboratory, OLLE HEINONEN, Argonne National Laboratory — Doped Mott insulators are of particular interest in thin film magnetic heterostructures and high temperature superconductivity. Due to the strong contribution of electronic correlations in such systems, traditional electronic structure methods fail to predict or even just reproduce their properties. Since the late 40s, NiO was intensively studied as a prototypical Mott insulator. However, most of the theoretical studies depending on Density Functional Theory failed to reproduce all of NiO properties and were unable to predict the properties of the system in the presence of defects. Quantum Monte Carlo (QMC) is a many-body quantum theory solving explicitly the electronic correlations, allowing reproducing and predicting materials properties with a limited number of controlled approximations. In this study, we investigate the energetics and properties of a pure bulk phase NiO and K-doped NiO semiconductor using QMC. Our results are then compared to a wide range of DFT approximations including SIC-DFT, DFT+U, hvbrid-DFT.

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