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First-principles analysis of magnetic interaction in electron-doped EuO JOONHEE AN, KIRILL BELASHCHENKO, University of Nebraska, Lincoln, KIRILL BELASHCHENKO'S GROUP TEAM — Using linear response calculations within the linear muffin-tin orbital method, we analyze the exchange interaction in electron-doped EuO. The 4f shell is treated within the LDA+U method. Calculations in the virtual crystal approximation show that the RKKY interaction mediated by the conduction band qualitatively explains the observed doping dependence of the Curie temperature in EuO. Further, to understand the role of a particular rare earth dopant, we consider EuO supercells with a substitutional Gd atom, as well as with an oxygen vacancy. Important differences with the virtual crystal approximation are found. The behavior of the exchange interaction in real space is analyzed, and its mechanisms are sorted out. The applicability of the magnetic polaron picture to Gd-doped EuO is evaluated.

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