Unconventional pairing states based on first principles

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We have combined the relativistic spin-polarized version of Korringa-Kohn-Rostoker method for the solution of the Dirac-Bogoliubov-de Gennes equations with a semi-phenomenological parametrization of the pairing interaction. We employ this method to both $LaNiGa_2$ and its non-centrosymmetric relative $LaNiC_2$ which show spontaneous magnetism in the superconducting state. Based on symmetry considerations it was already shown that the breaking of time-reversal symmetry is only compatible with non-unitary triplet pairing states in these crystals. Our method allows to study different on-site triplet equal-spin pairing models involving the first-principles band structure. We compare our predictions for the temperature dependence of the specific heat and it is found that it can be described by an interorbital equal-spin pairing on the nickel which breaks the time-reversal symmetry. It is shown that this pairing induces nodeless, two-gapped quasiparticle spectrum and finite magnetisation due to the redistribution of Cooper pairs in spin space. The method is also applied to Nb/Au/Fe multilayer system where we show that the existence of spin-polarized quantum well states can lead to FFLO-like oscillations of the order parameter in the normal metal.

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