Zero-bias peak induced by a magnetic impurity in a conventional superconductor: first principles-based study

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Topological superconductivity has emerged a promising platform for fault-tolerant quantum computing using braiding of Majorana modes. Considering that intrinsic topological superconductors are rare, various heterostructures including s-wave superconductors have been proposed to realize topological superconductivity. One of the viable heterostructures consists of ferromagnetic chains on conventional superconductors. Here we present our first-principles based study of a single magnetic impurity at the surface of an s-wave superconductor by solving the Bogoliubov-de Gennes equations for embedded impurity clusters within the screened Korringa-Kohn-Rostoker method in the framework of density-functional theory. We investigate the local density of states or bound Yu-Shiba-Rusinov states within the superconducting gap by varying the location of the magnetic impurity, the magnitude and direction of the magnetic moment, and spin-orbit coupling. Interestingly, we find a zero-energy peak near the single magnetic impurity with a judicious choice of environmental factors which may be observable in experiment.

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