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Simple Impurity Embedded in a Spherical Jellium: Approximations of Density Functional Theory compared to Quantum Monte Carlo Benchmarks MICHAL BAJDICH, MSTD, ORNL, Oak Ridge, TN 37831, JEOGNIM KIM, NCSA, UIUC, Urbana, IL 61801, USA, PAUL R.C. KENT, CNMS, ORNL, Oak Ridge, TN 37831, FERNANDO A. REBOREDO, MSTD, ORNL, Oak Ridge, TN 37831 — We study the electronic structure of a simple Gaussian impurity embedded in a spherical jellium in order to mimic the localization effects present in d- and f-electron compounds. We use quantum Monte Carlo benchmarks to validate approximations of density functional theory (DFT), such as local density approximation (LDA) and generalized gradient approximation (GGA) as well as the Hartree–Fock (HF) method. We identify distinct transitions between delocalized and localized states in the phase space of realistic densities ($1 \leq r_s \leq 5$) and moderate depths of the Gaussian impurity. We also extend the previous fixed-node diffusion Monte Carlo calculations of impurity-free jellium spheres and extract very accurate jellium surface exchange-correlation energies. Computer resources supported by DOE, Office of Science under contract DE-AC05-00OR22725 (NCCS). Research sponsored by DOE, BES, Materials Sciences and Engineering Division (FAR) and LDRD program (MB) and DOE SUF, CNMS (PRCK).

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