Energies and density distributions of $(^4He)_N$ clusters doped with $Br_2(X)$: A Hartree-like approach

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Energies and density distributions of the helium atoms in $Br_2(X)$-$(^4He)_N$ clusters are calculated using a quantum "Hartree-like" approach in which the dopant molecule and the ^4He atoms play the role of the nuclei and electrons, respectively, of the original Hartree formulation. A detailed generalization of the methodology is presented. The validity of this treatment is assessed by comparing energies and density distributions for $N=2$ up to $N=18$ with those obtained by performing quantum diffusion Monte Carlo (DMC) calculations. The present Hartree model shows good agreement with the DMC calculations, the main difference being that the DMC density distributions of the He atoms are more isotropic than those generated via the model. The treatment is extended to larger (up to $N=60$) clusters and saturation effects are analyzed and discussed.