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Construction of adiabatic connection curve for electron-hole system using multicomponent Levy-Lieb Lagrangian JENNIFER ELWARD, BENJAMIN KAPLAN, ARINDAM CHAKRABORTY, Syracuse University — The electron-hole adiabatic connection curve (eh-ACC) is central in development of accurate correlation functional for multicomponent electron-hole density functional theory (eh-DFT). The construction of accurate eh-ACC is challenging because it requires density constrained energy minimization at different values of coupling constants. In the present work, the density constraint was avoided by defining an electron-hole Levy-Lieb Lagrangian (eh-LLL). For a given set of input electron and hole densities, the eh-LLL was constructed and expressed as a functional of the coupling constant dependent external potential. Unconstrained minimization of the eh-LLL was performed by varying the eh-wavefunction, external potential, and Lagrange's multipliers. An explicitly correlated ansatz was used for the eh-wavefunction and the search over the wavefunction was performed using variational Monte Carlo. The calculation was repeated for coupling constants in the range of 0 to 1 and the minimized wavefunction was used for construction of the eh-ACC. This study represents the first step in construction of accurate electron-hole correlation functional for eh-DFT.

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