

A correlation energy functional from a correlation factor model

Fuentealba,

In this work, a way to approximate the correlation energy functional starting from a model correlation factor is shown. The problem is addressed by using formally exact properties of the second-order density matrix and actual values of correlation energies for atoms. An Ansatz for the correlation factor is proposed that allows one to derive some known and some new correlation energy density functionals. Results for atomic systems show the reliability of the approach. © 1994 John Wiley & Sons, Inc. Copyright © 1994 John Wiley & Sons, Inc.