Visualizing Molecular Wavefunctions Using Monte Carlo Methods

STEVE ALEXANDER, Southwestern University, R.L. COLDWELL, Retired

— Using a grid of up to 65 machines and variational Monte Carlo methods we have calculated the electron density, the intracule density, the extracule density, the electron density difference, two versions of the kinetic energy density, the Laplacian of the electron density, the Laplacian of the intracule density and the Laplacian of the extracule density of the ground state of H\textsubscript{2}, Li\textsubscript{2}, Be\textsubscript{2}, B\textsubscript{2}, C\textsubscript{2}, N\textsubscript{2}, O\textsubscript{2}, and F\textsubscript{2} near their equilibrium distance. We discuss how contour plots of these properties can be used to visualize the distributions of electrons in each molecule.