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Visualizing the Hydrogen Molecule Using Monte Carlo Methods
S.A. ALEXANDER, Southwestern University, SUMITA DATTA, S.N. Bose National Centre for Basic Sciences, R.L. COLDWELL, University of Florida — Many concepts in chemistry are based on localized groups of electrons (e.g. atomic shells, binding and lone pairs, π and σ electrons). These concepts have been related to the results of quantum mechanical calculations through a wide variety of atomic and molecular functions. Using explicitly correlated wavefunctions and variational Monte Carlo we calculate the electron density, the electron density difference, the intracule density, the extracule density, two forms of the kinetic energy density, the Laplacian of the electron density, the Laplacian of the intracule density and the Laplacian of the extracule density on a dense grid of points for the ground state of the hydrogen molecule with symmetry $X^1\Sigma_g^+$, $B^1\Sigma_u^+$, $a^3\Sigma_g^+$, $b^3\Sigma_u^+$, $I^1\Pi_g$, $C^1\Pi_u$, $i^3\Pi_g$, $c^3\Pi_u$, $J^1\Delta_g$ and $j^3\Delta_g$. With these values we construct a contour plot of each function and describe how it can be used to visualize the distribution of electrons in this molecule.

S.A. Alexander
Southwestern University

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