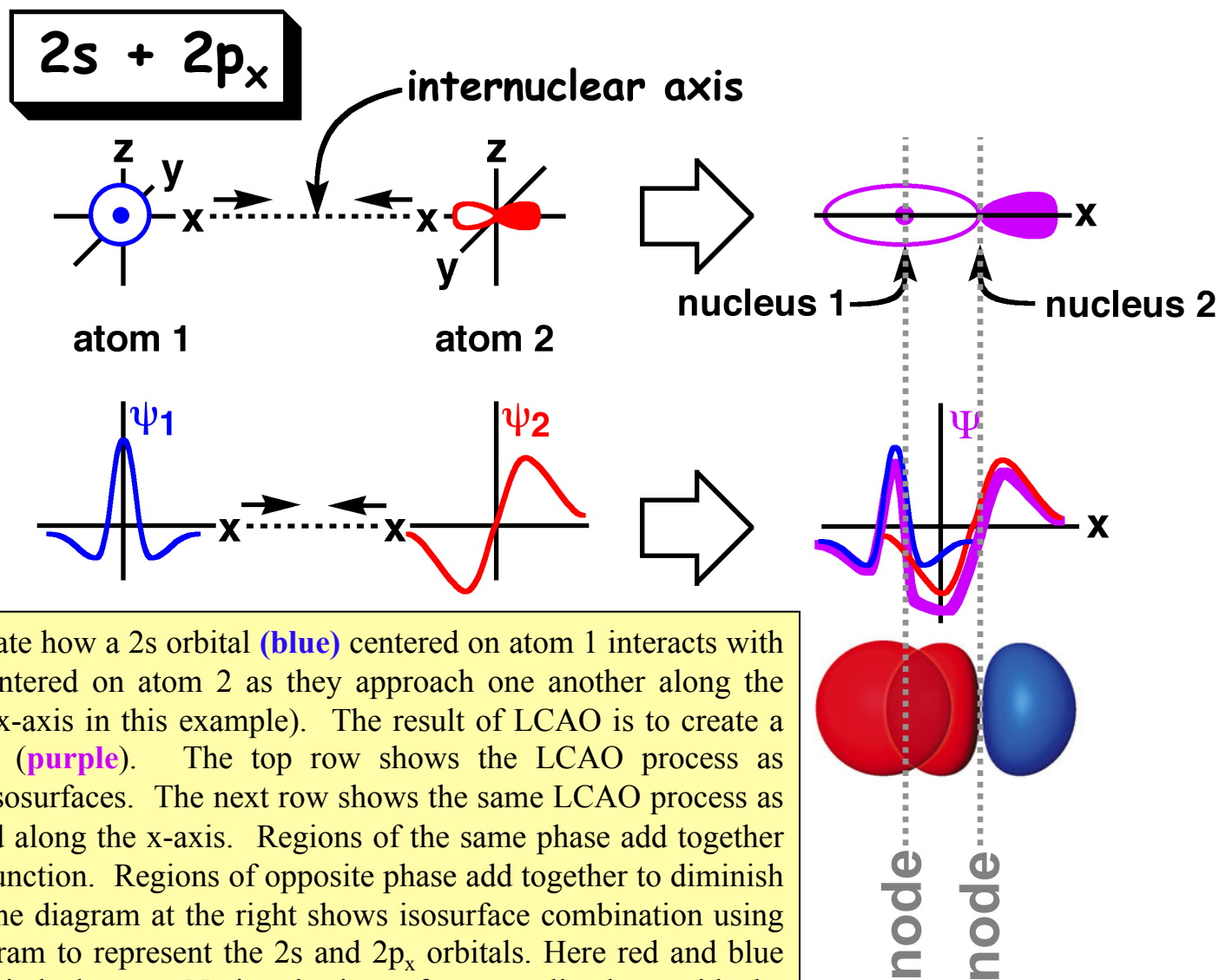


Linear Combination of Atomic Orbitals (LCAO)



These diagrams illustrate how a 2s orbital (blue) centered on atom 1 interacts with a $2p_x$ orbital (red) centered on atom 2 as they approach one another along the internuclear axis (the x-axis in this example). The result of LCAO is to create a new MO called Ψ (purple). The top row shows the LCAO process as schematically drawn isosurfaces. The next row shows the same LCAO process as wave functions plotted along the x-axis. Regions of the same phase add together to enhance the wave function. Regions of opposite phase add together to diminish the wave function. The diagram at the right shows isosurface combination using modern graphics program to represent the 2s and $2p_x$ orbitals. Here red and blue represent different orbital phases. Notice the isosurfaces are lined up with the diagrams of Ψ above; notice also how the nodes line up with the nuclei and notice that there is reinforcement of Ψ between the nuclei.

