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Accelerating self consistent field convergence by rubber sheeting of initial electronic wave functions. G. ERIC MATTHEWS, N.A.W. HOLZWARTH, GEORGE MARTIN, BRIANA KEELING, DOUGLAS AGOP-SOWICZ, Wake Forest University — We develop an algorithm for generating better initial electronic wave function estimates for density functional theory calculations following atomic movement. First principles molecular dynamics and atomic relaxation calculations involve successive movements of atoms followed by self consistent field (SCF) solutions for electronic wave functions. The SCF solutions converge most rapidly when starting from reasonably good estimates. Often estimates are generated directly from the wave functions of the previous atomic positions without adjustments for effects of position changes. Such estimates result in fast convergence to the correct wave function for small atomic movements, but for larger movements, convergence may be much slower. We present a method for improving the estimates of the new wave functions by using information from the movement of the atoms. Our algorithm is based on the “rubber-sheeting” method used in overlaying satellite imagery on geographic maps. A warping function is calculated that stretches and shrinks different regions of the wave function so that regions near nuclei are dragged along with the atoms. These estimates yield faster convergence for cases studied thus far.

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