Smooth exchange-correlation potentials from electron densities

ALEX P. GAIDUK, University of California, Davis, ILYA G. RYABINKIN, University of Toronto Scarborough, VIKTOR N. STAROVEROV, University of Western Ontario — Kohn–Sham potentials reconstructed from electron densities in finite basis sets often contain unphysical oscillations and asymptotic divergences which affect the properties computed with such potentials. We noticed that these artifacts are determined by the basis set in which the density is expanded, and are almost independent of the approximation used for computing the density. Guided by this observation, we developed a simple procedure for improving the shape of reconstructed potentials. Our scheme consists in computing an oscillation profile for a given basis set using a known exchange-correlation potential and subtracting it from the reconstructed potential of interest. Our correction leads to significant improvement of the shape of potentials and properties computed with them.

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Date submitted: 14 Nov 2013   Electronic form version 1.4