

Abstract Submitted
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System-averaged exchange and correlation holes in third-row atoms ANTONIO C. CANCIO, Ball State University — Recent work is presented on the theoretical calculation of system-averaged exchange and correlation holes (intracules) for a pseudopotential model of the valence shell of third-row atoms. Exchange holes are obtained from numerical fourier transform methods and correlation holes from variational quantum Monte Carlo calculations using the method of correlated estimates. We observe approximate scaling behavior in both exchange and correlation, following the known scaling of the valence density across the row. The holes are compared to density-functional models including LDA, GGA and meta-GGA approaches. Particular attention is paid to self interaction (SI) error; we find that a sizeable error occurs in the same-spin channel of the correlation hole which persists for the LDA and GGA even after standard SI corrections are applied. A simple SI correction that eliminates this error will be discussed.

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