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System-averaged exchange-correlation holes and self interaction in second-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 for the second row atoms Mg through Ar. 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 scaling behavior in both exchange and correlation, following the known scaling of the valence density across the row, once self-interaction effects are taken into account. The holes are compared to density-functional models including LDA, GGA and related SIC approaches. We note a sizeable error due to self-interaction occurs in the same-spin channel of the correlation hole which persists for the LDA and GGA even after standard self-interaction corrections are applied. The effects of this error and proposed corrections to it on the total exchange-correlation energy will be discussed.

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