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Spherically and system-averaged pair densities in the strong-interaction limit of density functional theory PAOLA GORI-GIORGI, ANDREAS SAVIN, Laboratoire Chimie Theorique, CNRS and University Paris VI, Paris, France, MICHAEL SEIDL, Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany — The spherically and system-averaged pair density (also known in chemistry as intracule density) plays a central role in the construction and understanding of exchange-correlation energy functionals in density functional theory. We have calculated the intracule density for several atoms in the strong-interaction limit of density functional theory. Comparison of our results with the same quantities calculated in the opposite limit, the non-interacting Kohn-Sham system, provides useful insight on the nature of electronic correlation in density functional theory.

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