

# Atomic spin-density polarization index and atomic spin-density information entropy distance

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It is shown that information theory concepts based on the Shannon entropy are useful to define indices yielding a quantitative measure of spin polarization. Numerical results for the ground state of all the atoms from He to Xe are presented. They were obtained by solving numerically the Kohn-Sham equations with two different approximations for the exchange-correlation functionals. The defined indices predict very nicely the periodical trends along the periodical table of elements. They are numerically great for atoms with the greater spin multiplicity and zero for closed-shell atoms. © 2002 Wiley Periodicals, Inc. *Int. J. Quantum Chem.*