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Practical method for calculation of the chemical reactivity indices
applicable in the conceptual DFT theory.

<u>Summary of the doctoral thesis</u>

The dissertation describes the implementation of a research goal focusing on finding a computational method for reactivity measures such as local softness, the Fukui function and global hardness, based on electron density functions, beyond the finite difference approximation. An attempt was made to use this knowledge to predict changes in thermodynamic functions as a result of reactions. The gradient theorem was used, opening a direct connection between the electron density function of the tested object and the local softness, without the need to differentiate by the number of electrons N. A working formula leading to the local softness is presented, which is the rational approximation justified by the principle of nearsightedness for electronic matter, NEM. By applying the above method to atoms, it has been demonstrated to be useful in easily accessing otherwise unobtainable quantitative softness data (local and global) for atoms and ions. The basic prediction results are presented in the form of radial distributions of local softness and the Fukui functions. This opened the way to the calculation of higher derivatives of the electron density and thus reactivity indices. The developed method was also used to analyse density derivatives described by hydrogen-like orbitals, which allowed, among others, to reveal the dependence of global softness on the atomic number of the nucleus. Results for the first and second derivatives of the electron density with respect to N (number of electrons) and μ (chemical potential) are shown. The results were used to calculate changes in the state functions ΔN, ΔE and $\Delta \mu$ perturbed by a change in the external potential $\Delta v(\mathbf{r})$. It has been proven that local softness and local hypersoftness provide key chemical information on the sensitivity of the orbital density to the disturbance of the external potential $\Delta v(\mathbf{r})$, leading to the exchange of electrons ΔN and the corresponding changes in the state functions ΔE, $\Delta \mu$.