Atom-Condensed Density Functional Theory Chemical Concepts obtained through Analytical Methodologies

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Chemical concepts from Density Functional Theory have been highly successful in the scrutiny of atomic, molecular and solid-state properties and chemical reactivity.[1] The majority of these concepts are introduced as response functions of the system's energy E with respect to changes in the number of electrons N, the external potential $v(\mathbf{r})$ or both. These definitions have afforded the non-empirical calculation of these reactivity indices and applications in many fields of chemistry have been studied. Many of the computed values of these indices have been obtained using the so-called finite difference approach.

We now present an analytical approach to obtain these concepts up to the second order. Attention in this talk will be focused on the atom-condensed version of these (analytical) reactivity indices and their use in chemical interpretation.[2,3]

[1] (a) Parr, R. G.; Yang, W. *Annu. Rev. Phys. Chem*. **1995**, *46*, 701-728. (b) Chermette, H. *J. Comput. Chem.* **1999**, *20*, 129-154. (c) Geerlings, P.; De Proft, F.; Langenaeker, W. *Chem. Rev.* **2003**, *103*, 1793-1874. (d) Ayers, P. W.; Anderson, J. S. M.; Bartolotti, L. J. *Int. J. Quantum Chem.* **2005**, *101*, 520-534. (e) Liu, S. *Conceptual Density Functional Theory: Towards a New Chemical Reactivity Theory*; Wiley-VCH, 2022.

[2] Wang, B.; Geerlings, P.; Van Alsenoy, C.; Heidar-Zadeh, F.; Ayers, P. W.; De Proft, F. *J. Chem. Theory Comput.* **2023**, *19*, 3223-3236.

[3] Wang, B.; Geerlings, P.; Liu, S.; De Proft, F., submitted.