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Calculation of functional derivatives with respect to the external potential NICK SABLON, TIM FIEVEZ, FRANK DE PROFT, PAUL W. AYERS, PAUL GEERLINGS, Vrije Universiteit Brussel — Apart from its many computational advantages, density functional theory (DFT) presents a conceptual framework for the reactivity and stability interpretation of chemical systems. The central idea is to identify chemical concepts with first and higher order (functional) derivatives of the electronic energy with respect to the number of electrons N and the external potential $v(r)$. The local interpretation of chemical reactivity is generally done with the Fukui function and the dual descriptor. These reactivity indices are usually calculated by a finite difference approach, which is entirely justified in an exact theory. Practical DFT calculations make however use of approximate exchange-correlation functionals for which the DFT concepts can only correctly be obtained by an effective evaluation of the electronic energy derivatives. A recent methodology for the calculation of functional derivatives with respect to $v(r)$ is presented.^{1,2} Results are shown for a wide range of molecules among which substituted benzenes. A reactivity description of the alkaline earth oxides' (100) surface is expounded on as well.

¹P.W. Ayers, F. De Proft, A. Borgoo and P. Geerlings, J. Chem. Phys. 126, 224107 (2007).

²T. Fievez, N. Sablon, F. De Proft, P.W. Ayers and P. Geerlings, J. Chem. Theory Comput. 4, 1065 (2008).

Nick Sablon
Vrije Universiteit Brussel

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