

Chemical Reactivity of Ground and Excited States as Probed through Density Functional Theory Based Reactivity Indices

Conceptual Density Functional Theory (CDFT)^[1] has emerged as a very successful theory of chemical reactivity. In CDFT, chemical reactivity is probed through reactivity descriptors, response functions of the energy E of the system with respect to variations in either its number of electrons N , its external potential $v(\mathbf{r})$ or both. In addition, CDFT has provided the theoretical framework for reactivity principles, such as the hard and soft acids and bases principle. The CDFT reactivity index definitions have afforded the possibility for their non-empirical evaluation and applications in many fields of chemistry have been studied.

The larger part of these studies involved the finite difference approach to evaluate the reactivity descriptors. In this lecture, an analytical approach to CDFT will be outlined.^[2-5] Quantities investigated include the chemical hardness, the Fukui function and the linear response function. In addition, the extension to Conceptual Density Matrix Functional Theory (CDMFT) is discussed.^[5] A recent approach to evaluate the indices from a machine learning approach is additionally highlighted.^[6]

In the final part of the lecture, we explore the CDFT chemical concepts and reactivity in excited states via the Δ SCF approach.

References

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Curriculum vitae of Prof. Dr. Frank De Proft

Frank De Proft is professor of theoretical and quantum chemistry at the Vrije Universiteit Brussel (VUB), directing the Research Group of General Chemistry (ALGC; <https://algc.research.vub.be>), the quantum chemistry group of the VUB.

After obtaining his Master's degree in Chemistry with a graduate thesis in synthetic organic chemistry, F. De Proft turned to theoretical chemistry for his PhD research in 1991, where he became interested in density functional theory.



Prof. Dr. Frank De Proft

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During his PhD studies, he was appointed as a predoctoral fellow at the Research Foundation-Flanders, Belgium (FWO). He obtained his PhD in Sciences at the VUB in 1995 and was appointed as FWO postdoctoral researcher from the period 1995-1999. In 1996, he conducted a postdoctoral stay in the group of Prof. Robert G. Parr (University of North Carolina at Chapel Hill, USA), a leading authority in the field of quantum chemistry and the founding father of conceptual DFT, funded by a Fulbright award for research and a NATO fellowship. In 1999, F. De Proft got tenure at the Vrije Universiteit Brussel. He was the 2007 Laureate of the Royal Flanders Academy of Sciences and Art in the Division of Natural Sciences. During his career, study visits were conducted, among others, in the group of Prof. Paul von Ragué Schleyer (University of Erlangen-Nürnberg, Germany) and Prof. David J. Tozer (Durham University, UK). In addition, he was twice invited professor in France [Université Pierre et Marie Curie, Paris (2006) and Université Claude Bernard Lyon 1 (2014)]. From 2016 to 2019, he was appointed as Francqui Research Professor.

Central in his research is the so-called “Conceptual Density Functional Theory” (CDFT) focusing on the development, implementation and computation of DFT based reactivity descriptors and concepts to gain insight into the reactivity of atoms, molecules and solids. His research strategy has always involved the coupling of this fundamental research line with a more applied part, situated in various domains of chemistry, ranging from inorganic via organic to biochemistry and catalysis, nearly always in direct collaboration with experimentalists.