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Editorial

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DFT Elucidation of Materials Properties

Just 50 years ago this November, Walter Kohn and Pierre Hohenberg published their theorem that laid the foundation of density functional theory, DFT. However, it is only some two decades ago that the introduction of modern gradient and hybrid density functionals brought DFT into general use by the chemistry community. From a practical standpoint, this advance occurred when the Pople group introduced these functionals and a robust, generally usable form of DFT into the Gaussian program in the mid-1990s. From that time on, the chemistry community became increasingly exposed to electronic-structure calculations based on Kohn–Sham density functional theory in addition to wave function and post-Hartree–Fock methodologies. These developments were in part responsible for the 1998 Nobel Prize in Chemistry being awarded to a mathematical chemist, John Pople, and to a theoretical physicist, Walter Kohn. The Prize also indirectly celebrated all those scientists memorialized in our modern acronyms for density functionals, like BLYP, PBE, and many others. (For a recent perspective on the development of DFT, please see the recent article of Axel Becke in the *Journal of Chemical Physics*[1]).

The use of DFT is now ubiquitous in the field of chemistry. There is not a current issue of the *Journal of the American Chemical Society* or other major chemistry journals without a number of articles in which DFT is exploited in a key or supporting role. This success is due largely to the computational efficiency of DFT and its explicit consideration of a great part of the electron correlation effects that are neglected by Hartree–Fock methods. A myriad of new codes is now routinely exploited in chemistry and chemical engineering departments, such as VASP, Turbomole, DMol, and ADF, to cite but a few.

The application of DFT to chemistry has meant the consideration of molecular systems, clusters, and materials in which the electron density varies widely and that interact noncovalently by, for instance, dispersion forces or hydrogen bonds. This has led, and continues to lead, to many efforts to improve density functionals, improvements that are meant to culminate in the holy grail of DFT: the development of the exact exchange-correlation potential.

Where DFT has definitely had a major impact is materials chemistry, and the subject featured in this Special Issue of *Accounts of Chemical Research* focuses on the "DFT Elucidation of Materials Properties". This is the first Special Issue of the journal where density functional theory plays the central role, and it is commemorated by the cover displaying Fang Liu's conception of the surfaces and clusters described here, along with the imaginative vision of ρ, the symbol of electron density upon which DFT is based, coalescing from small particles.

The Accounts included in the issue cover a wide range of topics, broadly devoted to the following:

- methodological aspects related to the description of dispersion interactions, interactions beyond van der Waals forces, or interactions between organic and inorganic components
- applications to spectroscopic, ferroelectric, charge, and spin transport or nonlinear optical properties of materials
- crystal-structure prediction
- chemical-engineering screening
- evaluation of organic (π-conjugated oligomers, graphene, fullerenes), inorganic (oxides, metals, intermetallic compounds), and hybrid organic–inorganic materials
- surfaces and interfaces

This Special Issue is intended to provide the chemistry community with a broad understanding of the current state-of-the-art in the application of density functional theory to materials and also to pave the way toward new advances in the use of DFT to elucidate and predict properties of new materials.

Jean-Luc Bredas, Guest Editor

King Abdullah University of Science & Technology

Kendall N. Houk, Senior Editor

University of California, Los Angeles

AUTHOR INFORMATION

Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

REFERENCES

(1) A. D. Becke, "Perspective: Fifty years of density-functional theory in chemical physics", J. Chem. Phys. 140, 18A301 (2014).

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