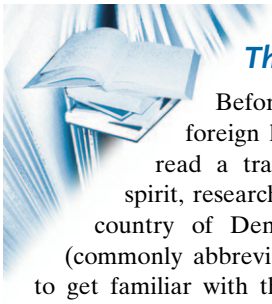

Density Functional Theory

Before making a journey to a foreign land it is a good idea to read a travel guide. In the same spirit, researchers planning to visit the country of Density Functional Theory (commonly abbreviated as DFT) may want to get familiar with the land of density functionals by reading the new book by David Sholl and Janice Steckel, who offer a tour for a first-time visitor to DFT, as well as brief guidance for the reader whom they call a quantum chemistry tourist. DFT was terra incognita until its discovery by Kohn and Hohenberg in the 1960s. More than 40 years later, this land has become a goldmine with numerous functionals that yield predictions of varying accuracy about the electronic structure of large and complex systems.

A question a prospective DFT traveler will probably ask is: why should he or she buy this particular book, when several other rough and smooth guides are already available on the market? (I stress here the words "prospective traveler", since the new book is clearly intended more for DFT greenhorns than for frequent flyers to DFT land or even natives.) One reason is that the book by Sholl and Steckel is easy to read, and it equips the traveler with the necessary (perhaps more than necessary) confidence for deciding on a DFT adventure and also with a basic survival kit. A very nice feature of this survival kit is that it contains numerous practical examples from life in DFT land and exercises by which one can train and acquire the skills needed to get through there. Moreover, the material in the survival kit is fresh, encompassing modern developments in functionals such as the inclusion of dispersion interactions, as well as containing a whole chapter devoted to ab initio molecular dynamics. The authors also spend a considerable amount of time on material that is not necessarily specific to DFT travels, but is relevant for any electronic structure method, including transition-state theory and vibrational analysis. Another reason why one may want to buy this book is connected with the fact that the land of DFT has two major regions—the Highlands, with the sharp hills and deep valleys of molecules and complexes, and the Lowlands, with the more gentle and regular landscape of periodic solid-state systems. Whereas there is already an excellent modern travel guide to the molecular Highlands by Koch and Holthausen, the solid-state Lowlands, on which the present book focuses, have until now only been covered by older, more vintage, texts.

The biggest single problem with the DFT guide by Sholl and Steckel is that it also aims to provide basic information about the neighboring lands of Hartree–Fock and other wavefunction-based methods. The authors are clearly well traveled in the DFT country, but commit the mistake of directly extending their experience to regions they have not explored so thoroughly. As a result, their introduction to the Hartree–Fock method is biased towards the DFT methodology, to the extent that some basic equations presented in Section 1.6 are not quite correct. Nevertheless, this book is a very useful and up-to-date guide to the land of DFT, in particular to the solid-state Lowlands, both for newcomers among students and for more senior researchers.

Pavel Jungwirth
Institute of Organic Chemistry and Biochemistry
Academy of Sciences of the Czech Republic
Prague (Czech Republic)

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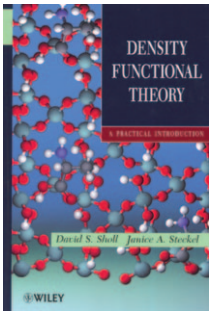

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