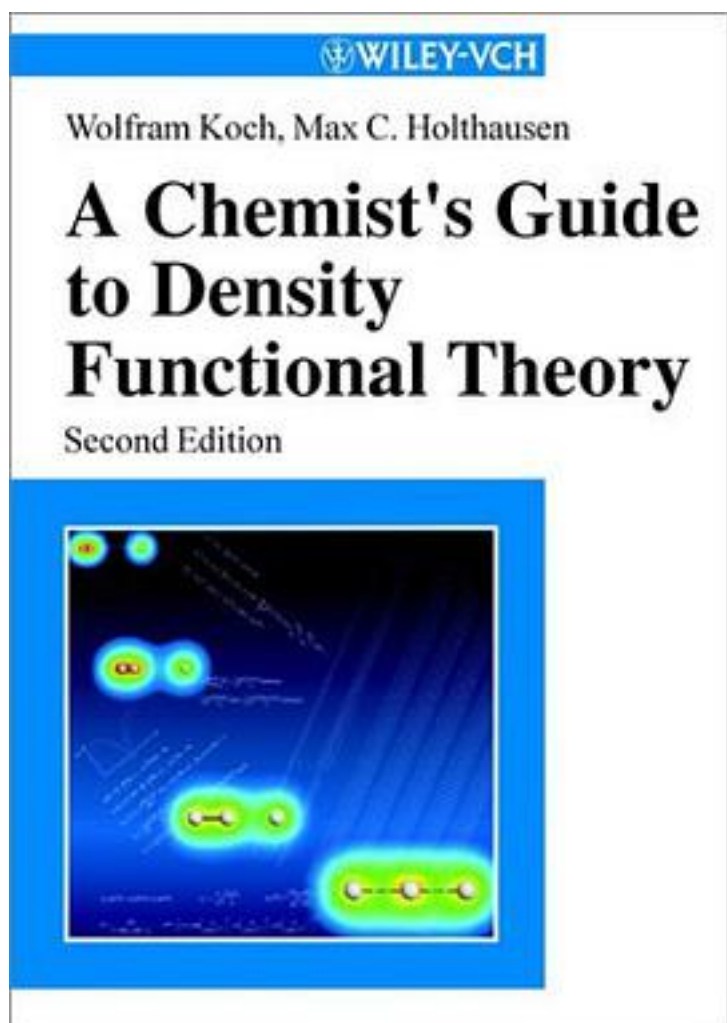


# A Chemist's Guide to Density Functional Theory, 2nd Edition



[A Chemist's Guide to Density Functional Theory, 2nd Edition\\_下载链接1](#)

著者:Wolfram Koch

出版者:Wiley-VCH

出版时间:2001-07-11

装帧:Paperback

isbn:9783527303724

"Chemists familiar with conventional quantum mechanics will applaud and benefit greatly from this particularly instructive, thorough and clearly written exposition of density functional theory: its basis, concepts, terms, implementation, and performance in diverse applications. Users of DFT for structure, energy, and molecular property computations, as well as reaction mechanism studies, are guided to the optimum choices of the most effective methods. Well done!"

Paul von Ragué Schleyer

"A conspicuous hole in the computational chemist's library is nicely filled by this book, which provides a wide-ranging and pragmatic view of the subject.[...It] should justifiably become the favorite text on the subject for practitioners who aim to use DFT to solve chemical problems."

J. F. Stanton, J. Am. Chem. Soc.

"The authors' aim is to guide the chemist through basic theoretical and related technical aspects of DFT at an easy-to-understand theoretical level. They succeed admirably."

P. C. H. Mitchell, Appl. Organomet. Chem.

"The authors have done an excellent service to the chemical community. [...] A Chemist's Guide to Density Functional Theory is exactly what the title suggests. It should be an invaluable source of insight and knowledge for many chemists using DFT approaches to solve chemical problems."

M. Kaupp, Angew. Chem.

作者介绍:

目录:

[A Chemist's Guide to Density Functional Theory, 2nd Edition\\_下载链接1](#)

标签

DFT

第一本书

量子化学

化学

1

QC

## 评论

感觉作者就在讲故事一样 易读 简洁

-----  
not worthy enough

-----  
被老板推荐的DFT书，适合化学系的人看。但是很多定义/概念讲的比较浅很多困惑无法理解。 物理系的同学还是看physicsts写的DFT书吧。

-----  
[A Chemist's Guide to Density Functional Theory, 2nd Edition\\_下载链接1](#)

## 书评

-----  
[A Chemist's Guide to Density Functional Theory, 2nd Edition\\_下载链接1](#)