



# **A New-Generation Density Functional: Towards Chemical Accuracy for Chemistry of Main Group Elements (SpringerBriefs in Molecular Science)**

*Igor Ying Zhang, Xin Xu*

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*A New-Generation Density Functional: Towards Chemical Accuracy for Chemistry of Main Group Elements* covers the most recent progress in the development of a new generation of density functional theory (DFT) for accurate descriptions of thermochemistry, thermochemical kinetics, and nonbonded interactions of main group molecules. In this book, the authors present the doubly hybrid density functionals (DHDFs), which dramatically improve the accuracy for predictions of critical properties by including the role of the virtual (unoccupied) orbitals. The authors not only discuss the theoretical bases of three classes of DHDFs but also demonstrate their performance using some well-established benchmarking data sets.

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