

Review of Aromaticity and Metal Clusters

Aromaticity and Metal Clusters. Edited by Pratim Kumar Chattaraj (Indian Institute of Technology, Kharagpur, India). From the series: Atoms, Molecules, and Clusters: Structure, Reactivity, and Dynamics. Edited by P. K. Chattaraj. CRC Press (an imprint of Taylor & Francis Group): Boca Raton, FL. 2010. xxii + 436 pp. \$149.95. ISBN 978-1-4398-1334-8.

be of great interest to those who are interested in the application of DFT theory to metal clusters and to all those who would like to search for and characterize metal clusters that are predicted to be particularly stable, i.e., aromatic.

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This book consists of 21 chapters devoted primarily to the aromatic character of metal clusters. However, the title of the book is misleading because its chapters are in fact essentially devoid of discussion of experiments pertaining to aromatic metal clusters. It is possible that this is due to the novelty of this field—only a few examples of known clusters have been fully characterized as “aromatic”. In my opinion, a more appropriate title might have been “DFT Studies on the Potential Aromatic Character of Metal Clusters”, since almost all chapters describe computational results, with the vast majority utilizing density functional theory.

In spite of the fact that the first three chapters are devoted entirely to the “definition” of aromaticity, a concept in chemistry that is very difficult to define precisely—Wiberg once referred to aromaticity as a “large fuzzy ball”—almost every chapter that follows presents the authors’ own view of this concept. It would have been appropriate for the editor to have instructed the authors not to “redefine” aromaticity in each chapter to avoid unnecessary repetition.

There is a tremendous variation in the length, topics covered, and quality of the chapters. Chapters 1–3 very nicely introduce the reader to the accepted definition(s) of aromaticity, how it might be measured, and how it might be applied to metal clusters. For a reader exploring the field of metal clusters, Chapter 3 is especially instructive. There are several short chapters; e.g., Chapter 5, “Using the Electron Localization Function to Measure Aromaticity,” is only seven pages long and is essentially a “rederivation” of the function of electron localization and its application to a C₃₂ fullerene. There are three chapters (8, 9, and 11) that seem to be out of place in the book, since they do not cover the subject announced by the title—even the term *aromaticity* does not occur anywhere in these chapters. Their coverage ranges from magnetism in small metal clusters (Chapter 8) to the computational study (primarily DFT) of the structures, energetics, and properties of sodium clusters (Chapters 9 and 11). It appears that the best and most interesting was saved for near the end! I found Chapters 13–16, 18, and 20 all to be excellent. Aromaticity is directly addressed in these chapters for main group elements (Chapters 13–16), uranium clusters (Chapter 18), and cyclic chalcogenides (Chapter 20). Finally, I do not understand why Chapter 21 was included in this collection of articles, since it includes a lengthy discussion about the aromaticity of phosphazenes but makes no mention of any metal.

In conclusion, this book covers, in general, the application of DFT theory to a wide range of metal clusters. It would certainly

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