

Preface

You are reading the next, most current volume of “Practical Aspects of Computational Chemistry” book series. Four volumes published since 2012 augmented by an initial book: the “Practical Aspects of Computational Chemistry” published in 2009 have established five volume series devoted to the various aspects of computational chemistry that we (Jerzy Leszczynski and Manoj Shukla) are pleased to bring to you over the last few years. This volume covers recent developments and current applications covering nanomaterials, hydrogen-bonded clusters, semiempirical local coupled-cluster theory, charge-transfer coupling, ro-vibrational energy levels, relativistic effects and quantum electrodynamics in chemistry, mechanochemistry, passivation on metal oxide surfaces, and nano-QSAR. The state-of-the-science research reviews covering the current volume are distributed in 12 chapters.

Chapter 1 contributed by Barysz provides an overview of applications of relativistic effects and quantum electrodynamics in solving chemical problems such as predicting reliable X-ray spectra. Chapter 2 discusses an efficient algorithm to locate global energy minima of hydrogen-bonded clusters containing up to 55 water molecules and is written by Kazachenko and Thakkar. In Chap. 3, Zakharov et al. have discussed the development and application of semiempirical coupled-cluster theory to calculate optical parameters such as polarizabilities and hyperpolarizabilities of fragments of conjugated polymers. Ramos et al. have reviewed methods to compute charge-transfer couplings efficiently and accurately in Chap. 4. Carington has reviewed methods to compute ro-vibrational energy levels of small polyatomic molecules in Chap. 5.

The effectively unpaired electron theory for singlet states and its application extending from diatomic to graphene nanoclusters have been reviewed by Luzanov in Chap. 6. Bobadilla and Seminario have discussed the application of computational chemistry methods in designing of carbon-based nanodevices in Chap. 7. There is a growing interest in the area of computational mechanochemistry and it has been reviewed by Dopieralski and Latajka in Chap. 8. The mechanisms of different types of Lewis acid–Lewis base interactions have been discussed in Chap. 9 by Grabowski and results of computational modeling of iodine-containing drugs

have been reviewed by Yuldasheva et al. in Chap. 10. Rybakov et al. have discussed atomistic modeling of Si(110) passivation by atomic layer deposition of Al_2O_3 in Chap. 11. The last chapter contributed by Toropov et al. deals with the development of nano-QSAR.

We would like to take this opportunity to thank all contributors for devoting their time and hard work to make this project a success. We acknowledge the excellent support from the Presidium of the European Academy of Science as well as Editors at Springer. Of course, many thanks go to our family and friends without their support the realization of the book would not have been possible.

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