

Preface

It is a matter of great pleasure to bring the current volume, *Practical Aspects of Computational Chemistry III*. Most of the contributors in this volume have participated in our annual International Conference “Conference on Current Trends in Computational Chemistry (CCTCC)”. This volume covers diverse applications of computational methods currently being used in various areas of science and technology. Current volume presents results of state-of-the-science research reviews distributed in the 12 chapters.

The very first chapter explores how computational chemistry methods can be reliably used to explain complicated experimental scanning tunneling microscopy (STM) observations, and this chapter has been contributed by Sonnet and Riedel. In the second chapter, Ivashchenko et al. have reviewed structures and properties of TiN-based heterostructures as revealed by quantum molecular dynamics simulation. Applications of plane-wave density functional theory (DFT) in understanding the complex surface phenomena on metallic surfaces have been detailed by Pushpa in the next chapter. On the other hand, in the fourth chapter, Nhat et al. have presented results of their investigation on geometries, electronic and energetic properties of vanadium doped gold cluster by considering up to 20 gold atoms and adsorption of carbon monoxide on these clusters.

Polyhedral oligomeric silsesquioxane (POSS) cage molecules have wide applications in the material science and catalysis. Contribution comprising POSS cage molecules by Rehman and Gwaltney at the DFT level is presented in the fifth chapter. The magnetic properties of single-walled carbon nanotubes as well as their cross-linking architectures are reviewed by Hagelberg et al. in the next chapter. Golbraikh et al. have discussed how various statistical criteria can be used to predict the modelability of a chemical data set for quantitative structure-activity relationship models in the seventh chapter. The free energy gradient method and its application unrevealing properties of system in solution have been reviewed by Georg et al. in the eighth chapter.

Hydrologic modeling approach to simulate pollution transport has been discussed by Pradhan et al. in the ninth chapter. On the other hand, Majumdar et al. have reviewed current status of research on nerve agents in the next chapter.

Storoniak et al. have discussed and reviewed the molecular factors governing the stability of the valence bound anions of DNA related system in the eleventh chapter. The last chapter reviewed by Wang et al. addresses a fundamental question of origin of life and how computational chemistry methods can play a vital role in addressing such an important question.

With great pleasure, we take this opportunity to thank all contributors for devoting their time and hard work to make this project a success. We are also thankful to all reviewers who devoted their time and efforts in providing valuable comments to each contribution in this volume. We are grateful for the excellent support from the Presidium of the European Academy of Sciences 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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