Book Reviews

Evolutionary Algorithms in Molecular Design. Methods and Principles in Medicinal Chemistry. Volume 8. Edited by David E. Clark (Aventis Pharma Ltd.; currently at Argenta Discovery Ltd., Dagenham, England). Wiley-VCH: Weinheim and New York. 2000. xii + 276 pp. $145. ISBN 3-527-30155-0

This book, which is part of a series organized by R. Mannhold, H. Kubinyi, and H. Timmerman, deals with an important approach used in computer-aided ligand design (CALD). The editor of this volume, David E. Clark, is one of the most respected authors in the CALD branch of computational chemistry. Among his contributions are two chapters in *Reviews in Computational Chemistry*: one on "Current Issues in De Novo Molecular Design" (1997) and one on "Computer-Aided Molecular Diversity Analysis and Combinatorial Library Design" (2000). Thus, he has broad, substantive basis for producing this book on evolutionary algorithms.

As stated in the preface, medicinal chemists have long used Darwinian principles, probably without realizing it, in their efforts to discover and optimize the bioactivity of new compounds. These chemists modify structures and combine various functional groups and templates, often in a random fashion, in an attempt to find iteratively the combination of structural components that will allow a molecule to survive the many tests and evaluative challenges before becoming a viable therapeutic agent. Clark's book is not about such implicit use of Darwinian principles, but rather it is about explicitly using computer algorithms designed to help chemists solve research problems.

The first chapter is a clear and simple description appropriately entitled "Introduction to Evolutionary Algorithms" (Abby Parrill). This chapter details the required knowledge to understand and use evolutionary algorithms. The final chapter, entitled "New Techniques and Future Directions" (Andrew Tuson and David Clark), presents the current stage of the evolutionary algorithms and describes developments that can be expected in the near future.

The other 10 chapters are dedicated to applications of evolutionary algorithms: "Small-molecule Geometry Optimization and Conformational Search" (Ron Wehrens), "Protein−Ligand Docking" (Garrett Morris, Arthur Olson, and David Goodsell), "De Novo Molecular Design" (Valerie Gillet), "Quantitative Structure−Activity Relationships" (Sung-Sau So), "Chemometrics" (Ron Wehrens and Lutgarde Buydens), "Chemical Structure Handling" (Peter Willett, who was Clark's Ph.D. director), "Molecular Diversity Analysis and Combinatorial Library Design" (Lutz Weber), "Evolutionary Algorithms in Crystallographic Applications" (Kenneth Harris, Roy Johnston, and Benson Kariuki), "Structure Determination by NMR Spectroscopy" (Bryan Sanctuary), and "Protein Folding" (Jan Pedersen). These chapters give a good overview of the broad utility of evolutionary algorithms. The contributors do not oversell evolutionary algorithms but rather offer an honest view of the advantages and disadvantages of them. Each chapter is fortified with a substantial number of references (many as recent as 1999) that allow the reader to delve more deeply into topics of interest.

The editor provides a one-page appendix giving Internet resources for evolutionary algorithms, and the book concludes with a 10-page subject index. The book's price is about 50 cents (U.S.) per page, which means that the publisher is targeting the book at a specialized audience.

We unequivocally recommend this book. The book is useful as a quick guide for employing evolutionary algorithms to a range of research problems, particularly those in CALD. In the jungle of the more than 1600 books that have been published on the many facets of computational chemistry, this volume is a natural selection.

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Solid State and Surface Photochemistry. Molecular and Supramolecular Photochemistry. Volume 5. By V. Ramamurthy (Tulane University) and Kirk S. Schanze (Florida State University). Marcel Dekker: New York and Basel. 2000. xii+328 pp. $333.33. ISBN 0-8247-0403-7

The mutually beneficial interaction between apparently disparate fields of science is seldom as productive and exciting as in the cases of solid-state and surface photochemistry. The collection of chapters presented in Volume 5 of *Molecular and Supramolecular Photochemistry* addresses the effects of solid-state surfaces and the bulk of crystalline solids on a wide variety of photophysical and photochemical molecular probes. The systems analyzed in this volume range from the diffusionless processes that occur in bulk molecular crystals of diarylethenes (Chapter 3) to cases that involve diffusion and transport. Examples of the latter include the gas−solid interfaces of silica gels (Chapter 1), the interstitial surfaces of clay materials (Chapter 2), and the intracrystalline channels of zeolite networks (Chapter 4−6). With the exception of photochemical reactions in molecular crystals, where the solid state has a relatively passive role, the common denominator between the various solid-state surfaces comes from the deep perturbations that the solid state causes to the ground and excited states of the molecules studied.

An introduction to the structure of each type of surface and a clear description of the techniques used to characterize them, which is included in almost every chapter of the book, should be welcomed by the reader. The effect of confinement by single crystalline solids on the photochromism of diarylethenes represents the system with the highest degree of structural information and is elegantly analyzed by Irie in Chapter 3. Solid-state systems analyzed in the other chapters have complex surface−adsorbate interactions characterized by a wide range of binding forces that have deep effects on their structures and equilibria. Perturbations to ground and excited states result in large spectral shifts and lifetime changes that can be correlated with experimental variables affecting the nature of surface−probe and probe−probe interactions. For instance, studies addressing the photodecomposition of polycyclic aromatic hydrocarbons (PAHs) on amorphous silica gel, by Dabestani and Sigman (Chapter 1), deal with the effects of adsorption at the gas−solid interface. It is shown that perturbations to ground and excited states come primarily from silanol−π-aromatic interactions, weak dispersion forces, and a highly heterogeneous surface, all of which restrict the diffusion of the probe, sometimes inducing its aggregation. The heterogeneous exposure of PAHs to gas molecules, including oxygen, is essential and advantageous for their photodegradation.

Other solid-state systems analyzed in Volume 5 are characterized by having higher degrees of order where the probe has lower molecular mobilities. For instance, intercalation of photoactive molecules within layers of clay oxides, or adsorption of probes along zeolite channels, results in specific probe−probe interactions that are determined by the crystalline structure of the solid host. The chapter by Takagi and Shichi (Chapter 2) is an excellent survey on the intercalation properties of clays, the photophysics of several well-known dyes, and the photochemistry of several inorganic and organic chromophores. The three chapters dealing with photochemistry and photophysics in zeolites have electron transfer and charge transfer processes as the main subject. A comprehensive review of a wide range of charge transfer complexes by Yoon (Chapter 4) should be an extremely valuable reference source. Hashimoto in Chapter 5 presents results from studies that are based on the detection of excited- and ground-state transients. The last chapter of the volume is a most welcomed and timely account of the work by Frei and collaborators on the very interesting area of zeolite-induced photo-oxidation with red light. This chapter addresses chemical, spectroscopic, and transient analysis of red-light photo-oxidation studies carried out by the authors, including evidence for charge-transfer interactions between hydrocarbons and molecular oxygen.

In summary, Volume 5 of *Molecular and Supramolecular Photochemistry* will be a useful source and reference book for the specialist and nonspecialist alike.

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