Catal Lett (2014) 144:1042
DOI 10.1007/s10562-014-1243-3

Aravind Asthagiri and Michael J Janik (eds): Computational Catalysis: RSC Catalysis Series (Royal Society of Chemistry)

ISBN: 978-1-84973-451-6, Copyright: 2013, Format: Hardback, Extent: 276, Price: $154

Rachel Getman

Received: 27 February 2014 / Accepted: 13 March 2014 / Published online: 30 March 2014

Graduate students, postdocs, research scientists, and professors in the field of computational catalysis will enjoy this anticipated book. It documents established and burgeoning computational and simulation methods for modeling heterogeneous catalysis, with an emphasis on metal catalysts. I have been modeling reactions over metal catalysts for nearly ten years, and I found the book to be thought provoking and useful. It provides detailed descriptions about activity descriptors, coverage effects, cluster expansions, the density derived electrostatic and chemical (DDEC) charge partitioning method, and effective bond orders (EBOs) and comprehensively documents methods for locating adsorption sites, deriving chemical potentials and other thermodynamic quantities from statistical mechanics, constructing scaling relationships and volcano plots, coding microkinetic models, simulating aqueous/metal interfaces for neutral and charged surfaces, and relating electrocatalyst surface potentials to various standard electrodes. To my knowledge, this is the first self-contained source to document many of these topics, making it a useful resource for students who are learning the field as well as for experienced researchers who want to cite the different methods using a single source. The descriptions are aimed to teach rather than to just review, which will be useful for people at all levels of the field of computational catalysis. That said, the book provides only a small tutorial on performing quantum chemical calculations, and thus I would recommend that newcomers use it in collaboration with a practical resource, such as *Density Functional Theory: A Practical Introduction* by David Sholl and Janice Steckel.

The book appropriately balances tutorials of established, state-of-the-art methods with discussions about growing areas of the field. In addition to the topics listed above, the book reviews the state-of-the-art in the growing field of activity at metal/support interfaces and describes some of the applications in the expanding area of using the ReaxFF and COMB force fields and molecular dynamics to model fluid/solid interfaces. The topics and case studies highlight cutting-edge research, and they have inspired me to think of new research ideas.

There are a number of growing subfields that are not extensively discussed, such as solvation models, stability analysis, and photocatalysis; however, the field of computational catalysis expands continuously, and discussing all of them would be intractable. That said, I hope to see a second and subsequent editions in 5–10 years that highlight new research areas and update the methods and strategies discussed in this edition.

This book provides a strong voice for computational catalysis and illustrates the care and scrutiny needed to construct and simulate models of catalytic systems. I recommend it to computational and experimental catalysis researchers alike.

R. Getman (✉)
Chemical and Biomolecular Engineering, Clemson University, Clemson, SC, USA
e-mail: rgetman@clemson.edu