

Preface

The use of computational methods has become an indispensable tool for elucidating the mechanism of organometallic reactions, including the mechanisms involved in catalysis by transition metals. The rapid increase in computer speed and the development of new computational methods and algorithmic improvements allow the study of the frequently complex reaction mechanisms in the important processes. As shown in this volume, the new developments in the field allow not only the study of systems such as clusters, which were previously out of reach for high-level calculations, but also see a shift from the rationalization of the mechanism towards more predictive models. We expect that this shift, which took place for purely organic molecules several years ago, will lead to an even stronger interest in the use of computational methods.

This volume contains a snapshot of the state of the art of computational studies of organometallic reactions, a field that has grown significantly and no single volume can attempt to provide a comprehensive overview. We therefore selected contributions in selected fields from authors in Asia, Europe, and the USA. The volume opens with a contribution by Yuxue Li on zirconium catalysis, a particularly timely topic in light of the award of the 2010 Nobel prize in Chemistry to Prof. Negishi, a pioneer in the synthetic application of these reactions. Marcus Meuwley reviews the use of force field methods in organometallic chemistry, which is a new and increasingly important method for the rapid studies of mechanism and selectivity in organometallic chemistry. The hydrogenation of π -systems is discussed in two contributions. Shuhua Li provides a broad overview of different mechanisms for the activation of molecular hydrogen. Forbes et al. discuss the rhodium, ruthenium, and iridium catalysis of this transformation, which is used in a number of large-scale production processes. Two further contributions discuss the oxidative functionalization of unactivated C–H bonds and of olefins. Xin Xu and coworkers provide an overview of the intensely studied field of alkane functionalization. The widely used osmylation reaction, for which computational methods played a crucial role in the determination of the now widely accepted reaction mechanism, is the topic of the contribution by Thomas Strassner and coworkers.

The use of molecular oxygen, a green oxidant, for oxidations through the use of transition metal clusters, is outlined by Zexing Cao. Clusters are also the topic of the contribution by Matthias Beller and Haijun Jiao, which demonstrates the interplay between experimental and computational methods that has been the hallmark of many studies in the field.

The breadth and depth of the contributions not only demonstrate the crucial role that computational methods play in the study of a wide range of organometallic reactions, but also attest to the robust health of the field that continues to benefit from, as well as inspire, novel experimental studies.

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