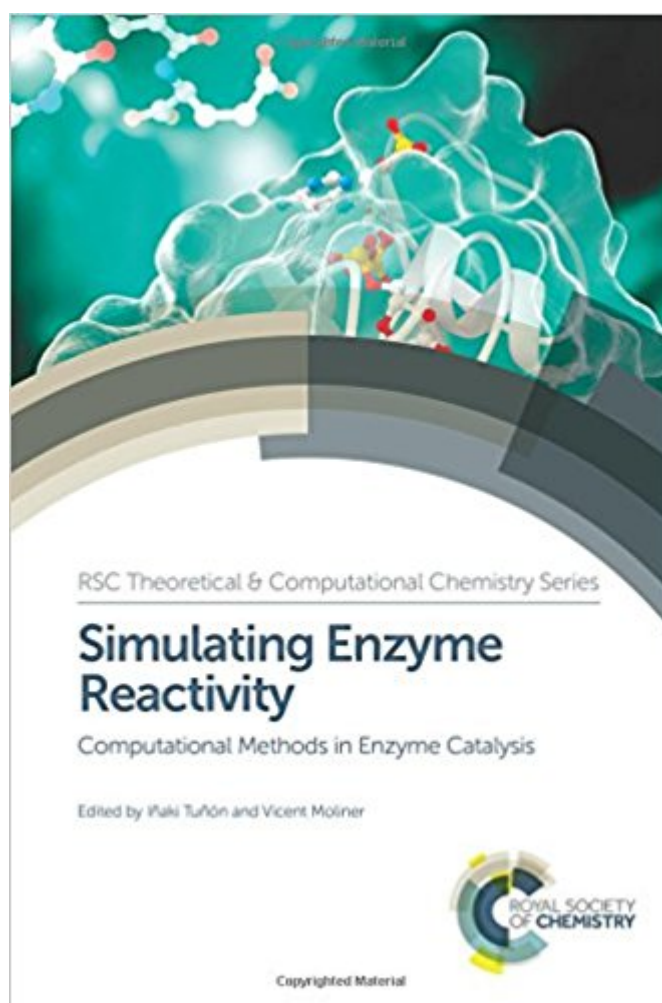


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The simulation of enzymatic processes is a well-established field within computational chemistry, as demonstrated by the 2013 Nobel Prize in Chemistry. It has been attracting increasing attention in recent years due to the potential applications in the development of new drugs or new environmental-friendly catalysts. Featuring contributions from renowned authors, including Nobel Laureate Arieh Warshel, this book explores the theories, methodologies and applications in simulations of enzyme reactions. It is the first book offering a comprehensive perspective of the field by examining several different methodological approaches and discussing their applicability and limitations. The book provides the basic knowledge for postgraduate students and researchers in chemistry, biochemistry and biophysics, who want a deeper understanding of complex biological process at the molecular level.

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