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Preface

Preface to proceedings of the symposium on methods and applications of combined quantum mechanical and molecular mechanical potentials (2001)

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The past decade saw remarkable progress in the development of combined quantum mechanical and molecular mechanical (QM/MM) methods and in the scope of their applications. This was mainly driven by the need to move quantum chemistry from the gas-phase realm to realistic applications in condensed phases and in biological systems. For these large molecular systems, it is not possible today or will not be possible even in the foreseeable future to carry out molecular dynamics simulations with sufficient sampling using reliable potential-energy surfaces fully described by ab initio molecular orbital theory and density functional theory. On the other hand, combined QM/MM methods offer the opportunity to perform QM calculations on truly large systems by dividing the system into a smaller region that is treated explicitly by quantum mechanics and a much larger portion of the system that is modeled by classical or molecular mechanics force fields. In this way, combined QM/MM methods take advantages of both computational accuracy and computational efficiency and, thus, have gained greater popularity.

The proceedings were developed from a symposium on Methods and Applications of Combined Quantum Mechanical and Molecular Mechanical Potentials at the 222nd American Chemical Society (ACS) National Meeting in Chicago, August 26–30, 2001. This is a sequel of a symposium on the same topics at the 214th ACS National Meeting in 1997. In a short period of 5 years, the field has grown to a much sophisticated level, ranging from technical issues, such as the treatment of the QM and MM boundary, to wider applications, such as enzyme catalysis. The breath and scope of this symposium are clearly reflected by the diverse topics covered by this volume.

We take this opportunity to thank all of the participants of our symposium and we look forward to future gatherings on this subject. We also would like to thank the editors of *Theoretical Chemistry Accounts* for making arrangements to publish these conference proceedings.

Contribution to the Proceedings of the Symposium on Combined QM/MM Methods at the 222nd National Meeting of the American Chemical Society, 2001

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