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More Realistic Molecular Modeling of Transition Metal Complexes with the Combined QM/MM and *ab initio* Molecular Dynamics Methods

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Computational chemistry is establishing itself as an invaluable tool for chemists of all disciplines. Despite the proven success of modeling in many areas of chemistry, its application towards studying transition metal based systems still presents a challenge for conventional techniques. Since transition metal based systems are a key component of many important industrial processes, a precise understanding of how these systems work is of significant scientific and commercial interest. Recently we have applied two novel computational techniques to examine transition metal complexes at the density functional level, namely, the combined quantum mechanics and molecular mechanics (QM/MM) method and the Car-Parrinello *ab initio* molecular dynamics methods. These two methods will be briefly introduced with a focus on how they can be utilized to build more realistic computational models than what is currently possible with traditional methods. Additionally, applications of the methods to study organometallic catalysts and complexes with extended ligand frameworks will be given.

Dr. Tom Woo has been an Assistant Professor in the Department of Chemistry at the University of Western Ontario since 2000. He obtained a B.Sc. in 1992 and a Ph.D. in 1998 from University of Calgary. He was then an NSERC Post-Doctoral Fellow at the ETH in Zürich, Switzerland in 1998-1999. His research interests lie in the area of theoretical and computational chemistry, with an emphasis on the development and application of quantum chemical techniques to investigate mechanistic aspects of catalytic processes. Dr. Woo has authored or co-authored about 30 journal articles and book chapters on the subject.