



Fall 2016 ACS COMP Symposium: QM/MM Simulation of Chemical and Biochemical Reaction Pathways: Recent Developments and Applications (252nd ACS National Meeting, August 21-25, 2016, Philadelphia, PA; organizers: Jingzhi Pu, Wei Yang, and Jiali Gao)

Combined quantum mechanical/molecular mechanical (QM/MM) simulation methods play a central role in mechanistic understanding of condensed phase reactive processes in complex chemical and biochemical systems. As is generally known, identifying reaction coordinates and mapping reaction pathways with proper statistical sampling are at the core of obtaining thermodynamic and kinetic information to provide mechanistic insights. However, the competing demand for highly accurate QM potentials and adequate statistical sampling has imposed an intrinsic constraint for the approach to be applied to very large-sized systems in a quantitatively reliable manner with commonly available computing resources. Recent years have witnessed exciting progress in both algorithmic developments and computing technologies, which offer promising new directions to tackle the related challenges. These advancements have set a new stage for applying QM/MM simulations to chemical/biological systems with ever increasing complexities. Through this symposium, we would like to gather the major scientists to summarize the progresses and discuss the remaining issues.

List of speakers:

Orlando Acevedo (U of Miami)
Victor Batista (Yale)
Andrés Cisneros (U of North Texas)
Qiang Cui (U of Wisconsin)
Colin Gaines (Rutgers)
Jiali Gao (U of Minnesota)
Sharon Hammes-Schiffer (UIUC)
Ming Huang (Rutgers)
Pengfei Huo (U of Rochester)
Hajime Hirao (Nanyang Tech U, Singapore)
Bill Jorgensen (Yale)
Gary Kedziora (Air Force Research Lab)
Hai Lin (U of Colorado Denver)
Dan Major (Bar-Ilan U, Israel)
Dmitry Morozov (U of Jyväskylä, Finland)
Kwangho Nam (U of Texas Arlington)

Jingzhi Pu (IUPUI)
Ursula Roethlisberger (EPFL, Switzerland)
Edina Rosta (King's College, UK)
Steven Schwartz (U of Arizona)
Yihan Shao (U of Oklahoma)
Lyudmila Slipchenko (Purdue)
Rui Sun (U of Chicago)
Walter Thiel (Max-Planck Institute, Germany)
Don Truhlar (U of Minnesota)
Iñaki Tuñón (U of Valencia, Spain)
Lee Woodcock (U of South Florida)
Weitao Yang (Duke)
Darrin York (Rutgers)
Yingkai Zhang (NYU)
Paul Zimmerman (U of Michigan)