

## **Brief Biographical Sketch Kenneth M. Merz Jr. Ph.D.**

Kenneth M. Merz, Jr. is currently a University Distinguished Professor, the Joseph Zichis Chair in Chemistry and a Professor of Biochemistry and Molecular Biology at Michigan State University. He was the Director of MSU's Institute for Cyber Enabled Research (iCER) from 2013-2019. Since the start of 2014, he has been the Editor-in-Chief of the Journal of Chemical Information and Modeling, which is part of the American Chemical Society suite of chemistry journals. His research interest lies in the development of theoretical and computational tools and their application to biological problems including structure and ligand based drug design, mechanistic enzymology and methodological verification and validation (*i.e.*, error analysis). In his research he makes extensive use of quantum and molecular mechanical potential functions coupled with a variety of numerical methods including molecular dynamics and Monte Carlo approaches. He also makes extensive use of structure-based drug design tools (*e.g.*, machine learning/AI) along with chemi and bioinformatics resources in his research program. He has also been heavily involved in software development (*e.g.*, parallel computing, GPU programming, *etc.*) aimed at taking advantage of high-performance computing (HPC) resources to solve chemical and biological problems. As a result of his research efforts, he has published over 300 papers and given over 300 lectures worldwide describing his research. Prior to his current position at Michigan State University he was a University of Florida Research Foundation Professor, the Edmund H. Prominski Professor of Chemistry, the Colonel Allan R. and Margaret G. Crow Term Professor and a Member of the Quantum Theory Project all at the University of Florida from 2005-2013. Prior to the University of Florida he was an Assistant, Associate and Professor of Chemistry at the Pennsylvania State University from 1989-2005. He also has worked in industry (1998-2001) first as the Senior Director of the Center for Informatics and Drug Discovery (CIDD) at Pharmacoepia, Inc. (now part of Ligand, Inc.) and then as the Senior Director of the ADMET Research and Development Group in the Accelrys software division of Pharmacoepia (now part of Dassault Systèmes and renamed BIOVIA). He is the founder of the software company QuantumBio, Inc and the Co-founder of the software company Attmos, Inc.. Dr. Merz carried out postdoctoral training at The University of California, San Francisco (1987-1989, with Peter Kollman) and at Cornell University (1986-1987, with Roald Hoffmann). He received his Ph.D. in Organic Chemistry at The University of Texas at Austin in 1985 (with M. J. S. Dewar) and his B.S. from Washington College, Chestertown, Maryland in 1981. He has received a number of honors including, election as the 2013 Chair of the COMP division of the ACS, election as an ACS Fellow, the 2010 ACS Award for Computers in Chemical and Pharmaceutical Research, election as a fellow of the American Association for the Advancement of Science, a John Simon Guggenheim Fellowship and he has held visiting professorships at Imperial College (London, England) the Institute for Research in Biomedicine (Barcelona, Spain), École Polytechnique (Paris, France), University of Florence (Florence, Italy), The University of Strasbourg (Strasbourg, France), The University of Oviedo (Oviedo, Spain) and the ETH (Zurich, Switzerland).