



Dr. Ralph A. Wheeler Professor and Chair of the Department of Chemistry and Biochemistry Duquesne University

Ralph Wheeler became a Professor and Chair of the Department of Chemistry and Biochemistry at Duquesne University in Pittsburgh in July 2010, after 20 years as a Professor in the Department of Chemistry and Biochemistry at the University of Oklahoma. Ralph received a BS in chemistry from Harvey Mudd College in 1982, a PhD in computational chemistry from Cornell University in 1988, and completed two years of postdoctoral training as an NIH Fellow with Andy McCammon in 1989. He rose through the academic ranks at the University of Oklahoma, winning three Junior Faculty Research Fellowships, a Regents' Award for Superior Research, and two American Chemical Society Awards for outstanding service. From 2003-2010, he held the title of Presidential Professor in recognition of outstanding research and mentoring. In 2010, Ralph was named a Fellow of the American Chemical Society to recognize his outstanding research and exceptional service. He served as Program Chair for the ACS Computers in Chemistry Division from 2000-2004 and the Division's Chair in 2007. He is currently serving his second term as an ACS Councilor, a member of the ACS Committee on Science, and its Policy Subcommittee.

His current research interests span computational biochemistry and materials chemistry, using quantum chemical, molecular dynamics, and QM/MM methods. They include developing new methods of finding global energy minima in condensed-phase structures and new ways to analyze dynamics simulations, primarily by adapting signal processing methods to predict vibrational spectra. His 75 publications have been cited more than 2600 times and most were co-authored by his 18 PhD/MS students and more than 32 undergraduate researchers. He is particularly proud of the many awards won by current and former students, including Fulbright, Goldwater, NIH, NSF, and National Research Council Fellowships, as well as an NSF POWRE Award (Professional Opportunities for Women in Research and Education).