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Theory and Modeling Group

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Larry Curtiss received his B.S. degree in Chemistry in 1969 from the University of Wisconsin-Madison and Ph.D. degree in Theoretical Chemistry in 1973 from Carnegie-Mellon University. He was a Battelle Institute Fellow at Battelle Memorial Institute in Columbus Ohio from 1973 to 1976. He joined the Chemical Engineering Division at Argonne National Laboratory in 1976. He was promoted to senior scientist in 1988 and to Distinguished Senior Scientist in 2000. He has been Group Leader of the Molecular Materials Group in the Materials Science and Chemistry Divisions since 1998. He has been serving as acting Group Leader for the CNM Theory and Modeling Group since 2006.

His research interest is in the area of computational chemistry including development of new quantum chemical methods and applications to problems in materials science and chemistry. Specific areas of interest include nanocatalysis, nanocrystalline materials, computational thermochemistry, electron transfer processes; and nanoporous materials. He has over 280 publications and numerous citations. He is listed as a Highly Cited Researcher by the Institute for Scientific Information (ISI) in Chemistry for the period 1980-1999. Among his awards and honors are the University of Chicago Distinguished Performance Award in 1995 the Fellow of the American Association for the Advancement of Science in 1997, and the Kilpatrick Lecture, Illinois Institute of Technology in 2000. He has served on review panels, is on the Executive Committee of the Institute for Energy and Catalytic Processes of Northwestern University and is on the editorial board of the Journal of Computational and Theoretical Nanoscience.

Larry Curtiss is widely known for his work in the development of quantum chemical methods and application of these methods. His methodology research at Argonne has focused on development of highly accurate quantum chemical methods for the calculation of energies such as bond energies, surface reaction energies, enthalpies of formation, electron affinities, and ionization energies that are important in modeling and simulation of materials properties. He has been at the forefront in developing quantum chemical approaches for accurate energy calculations. This has resulted in the successful Gaussian-n series (G1, G2, G3) and more recently G4 theory. With the availability of increasingly accurate experimental techniques for probing physical and chemical properties of materials at the atomic level, it is imperative to develop computational techniques to provide as accurate data as can be measured experimentally. His methodologies have been, and continue to be, extensively used in the research community in a wide range of applications. His papers on methodology development have received over 10,000 citations. Larry Curtiss is also known for his work in applications of electronic structure methods in areas such as catalysis, hydrogen bonding, electron transfer mechanisms, ion transport in polymer electrolytes for batteries, molten salts, catalysis, nanoparticles and diamond materials. Recently, he has contributed significantly to the fundamental understanding of ultrananocrystalline diamond (UNCD), a new form of diamond that was discovered at Argonne. By calculation of the potential energy surfaces of the molecular reactions on various surfaces of diamond, he was able to determine that the carbon dimer was the principal growth species and that, under the certain conditions, it can lead to nucleation of new diamond crystallites. Another current research area where his theoretical calculations on surface reactions have played an important part is catalysis. He has carried out extensive computational studies to understand catalytic reactions in zeolites and supported oxide surfaces.