William Andrew Goddard III

Over a career now spanning more than 50 years, Professor William ("Bill") Goddard's seminal contributions to theory and the application of theory and computation to the materials and chemical sciences have led to dramatic advances over a diverse range of fields within science and engineering. Never content to simply explain existing data or confirm experimental findings, Bill's bold predictions and insights have stimulated experimentalists in many communities to rethink their observations and design new experiments to test these predictions. Indeed, his advances have blurred the lines between theory, computation, and experiment, providing new thinking about how to manipulate nature to address the needs of humanity.

Bill began his scientific career as a graduate student in engineering science at Caltech, after receiving his B.S. in engineering with highest honors at UCLA in 1960. After finishing his Ph.D. in engineering science with a focus on materials science and physics in 1964, Bill joined the Chemistry and Chemical Engineering Division at Caltech as an Arthur Amos Noyes Research Fellow and studied how orbitals control the evolution of chemical reactions. After becoming a chemist and getting tenure in Chemistry, Bill's interests turned to surface science and semiconductors. and became a founding faculty member of the Applied Physics program at Caltech in 1970, where he developed the methodologies on surface science and how reconstruction of surfaces affect device electronic properties. Bill continues to be active in chemical, materials, and biological sciences and engineering and his passion for science is equally balanced with his ability to actively engage with his collaborators. His Materials and Process Simulation Center founded in 1990 has attracted a large and diverse set of students and researchers ranging from high school freshmen to professors and industrial scientists. Bill is truly an inspiration and is widely recognized for his sustained passion for science and his legacy in developing new theories and computational techniques and applying them to real problems.

Bill has epitomized Caltech in many ways: active and game-changing involvement in solving scientific and engineering problems using fundamental scientific principles. This is evident in how widely his theories and techniques have been or are being incorporated in some of the most widely used molecular simulation packages around the world. He has also been instrumental in commercial spin-offs (Materials Simulation Inc. now Accelrys and Schrödinger) that provide practical computational tools for materials and chemical design and for drug development that use principles that he pioneered to solve real-world challenges such as predicting 3D structures and activation of G protein-coupled receptors for such drug development activities as relieving pain without side effects. His legacy includes close integration of theory and experiments as we

move toward developing nanoscale devices that enable revolutionary applications in chemistry, materials science, and medicine.

Bill is an engineer among scientists and a scientist among engineers. His enthusiasm to explore new frontiers to boldly tackle problems beyond reasonable expectations is contagious. Over the past fifty years, the computing industry has followed Moore's law providing rapid expansion of computational capabilities that enabled the development and application of new techniques from Bill and collaborators aimed at expanding applications to chemical, materials, and biochemical systems to offer increasingly detailed understanding of their atomic level mechanisms, to provide the impetus as the engines of new designs. These advances in computation spurred the development of new methods and theories that have revolutionized the role of theory in materials and molecular science, enabling the design and discovery of new materials for the chemical, clean energy, materials, and drug industries. Bill's lifelong quest has been to develop theory and methodology that could drive applications to the new levels needed to enable theory to provide the basis for first principles-based macro-scale engineering design based on a hierarchy of overlapping paradigms that ultimately provide near quantum mechanical accuracy for predicting new materials for practical applications. Indeed, the US Government Materials Design and Materials Genome Initiatives since 2011 embody this philosophy of harnessing computational materials science, chemistry, and biology to provide the basis for reinventing manufacturing.