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Tribute to William Andrew Goddard III

Why do we honor Bill Goddard with this issue of *The Journal of Physical Chemistry?* It is not purely for the reason that he is one of the elite quantum chemists in the world. It is largely because of the gift that Bill has given to the scientific community: true *insight* from quantum chemistry—simple pictures from complex equations, not just numbers—and through his theories, especially the generalized valence bond theory, the foundations for chemical intuition.

Bill has never been content to simply explain existing data or to confirm experimental findings. No, Bill's favorite place to be is out on a limb, making an experimentally testable prediction. He has stimulated experimentalists in so many communities to go back and rethink their observations and to design new experiments to test his predictions. These include experimentalists working in the realms of gas phase chemical physics, solid state physics, surface science, polymer science, organometallic chemistry, and biochemistry, to name just a few.

We also honor him because he represents a unique personality in science. While many scientists are enthusiastic about their work, Bill goes beyond enthusiasm. He truly has a passionate love affair with scientific discovery. He does research because he cannot imagine doing anything else. He wants to know how the world works and he cannot wait to find out. It is not his ego; it is not chasing fame that drives Bill. It is his impression that there is not enough time in the day, in the week, in the month, in the year, ... to devote to discovery. One could describe him as a workaholic, although not in the sense of a compulsion. His insatiable drive is more like a fever, to uncover the mysteries of nature in the short time one has to live on this earth.

Bill started out his scientific life as an engineer, receiving his degree in that discipline from UCLA. He was a practical sort, reared by a migrant worker father and hard-working mother in the Imperial, San Joaquin, and Coachella valleys of California. His family moved often, living at about 35 different addresses before Bill turned 19. He was an only child, who attended more elementary and secondary schools than one can easily imagine, about 25 different ones by the 10th grade! We can trace the creativity and innovation that Bill has consistently exhibited in his work to his father, a crate-builder by trade, who figured out the most efficient way to build and distribute his crates. Young Bill was highly observant of his father's skill.

When Bill moved to Caltech for graduate school in Engineering Science, he began as an experimentalist. After a year and a half of experiments in materials science, he decided he was most interested in developing a conceptual understanding of why materials have the unique properties that they have. This led him directly to quantum mechanics, where he soon realized that, in order to predict properties of materials from the basic laws of physics, it would be necessary first to find practical means to solve the Schrödinger equation. His thesis work had little to do with materials science, and everything to do with quantum mechanics and many-electron wavefunctions.

He soon caught the attention of the Chemistry Department at Caltech, where Sunney Chan invited him to take on a Noyes Instructorship position. Bill is an original thinker, always thinking the practical means to the end, always going his own way in science. Bill's generalized valence bond theory, which applied the variational principle to valence bond wavefunctions, did so ultimately in a way that was simple to compute and offered tremendous qualitative insight into the electronic and geometric structures of molecules.

For many years, Bill worked primarily in the realm of molecular electronic structure, though he was one of the first to use cluster models to understand surface reconstructions and surface chemistry, and one of the first to develop ab initio based pseudopotentials or effective core potentials, as he referred to them. He was already thinking ahead to how he would ultimately investigate materials properties, by cheapening the cost of the calculation, by throwing away the core electrons, or by representing the solid surface by a cluster.

Bill created his Materials and Molecular Simulation Center at Caltech, in the late 1980s. This center, funded primarily by industrial contracts, originates from the thrill Bill gets from solving practical problems—the pragmatic in him revealed yet again. He now uses both his GVB methods, as well as other methods of simulation (molecular dynamics, Monte Carlo, etc.) with his own unique twists, to solve problems ranging from corrosion inhibition to catalysis to drug design. Many of Bill's graduate students leave Caltech, after receiving their Ph.D., thinking they should choose an area of research that does not overlap any of Bill's research areas. If they stay in the seemingly diverse range of theoretical physical sciences, they soon discover this to be an impossible task!

How will we think of Bill in the years to come? Well, beware: at his Festschrift banquet, when asked by his son when he planned to retire, he announced that he *might*—emphasis on the *might*—retire at 100!

Therefore, we can look forward to many more years of seeing Bill with his brightly colored beret (who can forget the bright green or yellow blazers he used to wear in 1980s?). Undoubt-

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edly, he will continue to come into seminars late, to occupy a front row seat, and to routinely fall asleep but still to wake up in time to add a cogent word or two to the discussion at the end. We can look forward to many more years of talks put together in the middle of the night or perhaps just before his own lecture during a conference. We can expect dense, hand-drawn viewgraphs and talks culled from too many slides, where we are always amazed that he pulls the proverbial rabbit out of the hat, such that we learn something highly original from each talk he gives. In addition, who can forget being the victim of his sudden questions during his own lecture, or his sudden involvement of you in an enactment of a dance of electrons? In his class on the Nature of the Chemical Bond, with the wondrously insightful, unpublished lecture notes that he wrote, he used to regularly employ the Socratic method. If you did not know the answer to a question, he said, "just say 'Duh'". Bill makes learning and scientific discovery FUN.

Those fortunate enough to be one of Bill's students will note other aspects of working with him. Students find that his mind can work like a dendritic polymer, where if you discuss one idea with him, he will put forth another ten. Students learn that he is not the most organized (!) of individuals and that once he understands the outcome of a calculation, he is ready to move on (and move the student on) to the next discovery, often without writing it up for publication. It takes tremendous discipline and force of will from the student to insist to Bill that he or she be allowed to take the time to write up the work at the time it is finished. Students also learn that it is impossible to work harder than Bill, at least over an extended period of time. Though he is a devoted family man (committed to his wife, four children, and eight grandchildren), he works 7 days a week, sleeping only four hours per night, consuming four 1-qt thermoses of coffee before noon, and then switching to caffeinated sodas.

The ultimate entropy generator, Bill runs from fire to fire, and it takes a unique secretary to keep him in water. He had a long-serving secretary, Adria McMillan, who sadly passed away a couple of years ago. She could make order out of chaos. His secretary must also be the one person who can reliably decode Bill's handwriting—the joke in the research group has been you cannot get your Ph.D. until you can read his handwriting. Undoubtedly, his secretaries in the post-Adria era have had and will continue to have their hands full.

Finally, in a more serious tone, all his students, past, present, and future, will note the caring that he exhibits toward each one. His philosophy is to bring out the best talents in each student or postdoctoral fellow, no matter what those talents might be. Bill recognizes that science is done by human beings, and human beings generally thrive on enthusiasm and positive feedback. He is a fountain of such enthusiasm and it is infectious. We look forward to him spreading his enthusiasm, his thrill of discovery, and his unique scientific insights well into the 21st century. Thank you, Bill, for what you have given our community.

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