Discovering the “Blue-Shift”

by Anna McEntire

Utah State University chemistry professor Steve Scheiner is the 2010 recipient of the D. Wynne Thorne Career Research Award, USU’s most prestigious faculty research accolade. He will give the keynote lecture at the faculty research awards luncheon, part of USU’s 2011 Research Week.

Scheiner is a computational chemist who uses quantum mechanics to understand the nature of interactions between molecules. His work is unusually broad, but his focus is hydrogen bonds, a chemical phenomenon fundamental to life itself.

“I consider Scheiner to be the world’s expert on the theoretical chemistry of hydrogen bonding, the molecular phenomena that accounts for the double helix of DNA, the activity of enzymes and that water is a liquid and paper a solid,” said Joel Liebman, professor of chemistry and biochemistry at the University of Maryland.

“Using quantum chemical methods, Dr. Scheiner has identified unique fingerprints of various hydrogen bonding interactions typically observed in bio-molecules,” said Joseph Francisco, professor of chemistry and Earth and atmospheric sciences at Purdue University and president of the American Chemical Society, a professional society of 162,000 members.

For a long time, chemists believed that hydrogen-bonded interactions could be identified by a distinctive “red-shift” of infrared light. Scheiner’s research, however, characterized a unique kind of hydrogen bond contact that emitted a “blue-shift.” His research further identified the origin of the phenomenon and focused on a previously overlooked hydrogen bond interaction, now known as the CH–O interaction.

“Scheiner’s book Hydrogen Bonding: A Theoretical Perspective has become the ‘Bible’ for theoretical studies in this area, the first place anyone turns who wants to work in this field,” said Paul Seybold, professor of chemistry and biochemistry at Wright State University. This book has been cited more than 1,000 times since its publication in 1997.

Scheiner received his doctorate in chemical physics from Harvard University in 1976. He held positions at The Ohio State University and Southern Illinois University, Carbondale before coming to Utah State in 2000. At USU, Scheiner served
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as the head of the chemistry and biochemistry department for nine years, from 2000 to 2009, while maintaining his active research program.

Scheiner’s research publications are prolific, with more than 250 peer-reviewed papers, ranging in disciplines from development of theoretical methodology to applications of quantum chemistry to many different areas of science. Just as important, though, is the rate at which other chemists cite his work in their own papers, which rivals leaders in the field at MIT, Stanford, Berkeley and Harvard. His work is cited some 400-500 times each year, and his H-index (a measure of scientific productivity and impact) has risen to 55.

“Steve was most highly rated by his peers partly because of his publications, but especially because of others’ citations of his work,” said Brent Miller, vice president for research at USU. “He has more than 250 publications, which have been cited an amazing 7,600 times. I think his citations are probably substantially higher than anyone at USU, and they reflect the broad impact of his work.”

Scheiner has been awarded more than $4.2 million in research grants, an unusually high amount for computational chemistry, said Alvan Hengge, head of USU’s chemistry and biochemistry department. His sponsors include the National Institutes of Health, the National Science Foundation, the Binational Science Foundation, Army Research Office and IBM.

Scheiner is frequently called on to review manuscripts prior to publication, reviewing some 100 manuscripts each year for more than 80 different scientific journals.

Throughout his research career, Scheiner has mentored numerous undergraduate and high school students, 12 doctoral students and 28 post docs.

Named after USU’s first vice president for research, the D. Wynne Thorne Career Research Award is given to an individual on the USU campus who has completed outstanding research in his or her career. The award is given annually to one outstanding university researcher who is recommended by a committee of peers, all previous award recipients. Nominees are evaluated for the significance and quality of their research and creative achievement, as well as recognition by national and international experts.