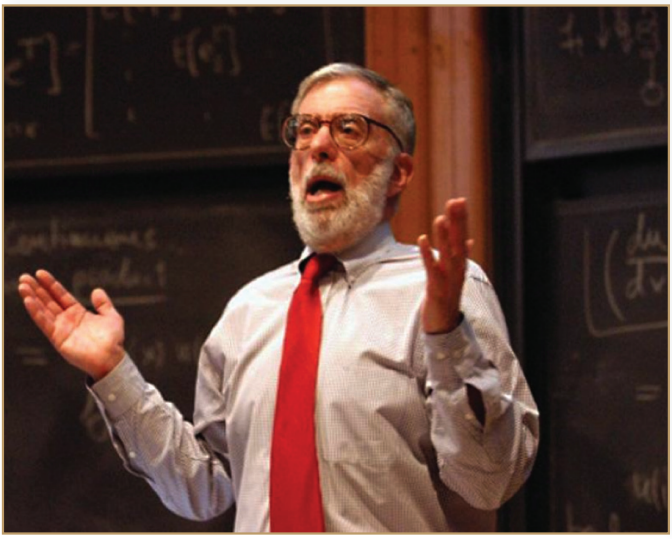


The Robert J. Silbey Memorial Symposium on Theory for Experimentalists

December 6-7, 2012

Georgia Tech Research Institute Conference Center
Atlanta, GA

… When he shall die
Take him and cut him out in little stars
And he will make the face of heaven so fine
That all the world will be in love with night
And pay no worship to the garish sun.

Romeo and Juliet, Act 3 scene 2

Biography of Robert J. Silbey

Written by Susan, Anna, and Jessica Silbey, and Sylvia Ceyer

Robert J. Silbey, Class of 1942 Professor of Chemistry, Dean of Science, and beloved teacher was born October 19, 1940. Raised in a lower middle class family in Brooklyn during and just after the Second World War, Bob was strongly influenced by the liberal atmosphere of that time and place. His father was the manager of a bottling plant on the Brooklyn docks; his mother worked at the Red Cross headquarters in New York City. He and his older brother by seven years, Joel, went to the public schools and then on to the public university system of New York City. Sidney Silbey had studied chemistry at Cooper Union in Manhattan, and Bob often commented that his early interest in chemistry probably stemmed from his father's interests and education. Like many young people of his generation, Bob owned a chemistry set he used to conduct experiments on the kitchen table, from time to time setting the table on fire. The Silbeys were not rich, but their apartment was richly filled with books, a fact that puzzled many childhood friends. Surrounded by piles of books since childhood, Bob was a voracious reader his entire life.

After graduating from Erasmus Hall High School, Bob went to City College to study chemical engineering. He had been accepted at several schools, including MIT, but the family could not afford the costs at the private institutions. Within six months at City College, however, Bob realized that he was more interested in chemistry and physics than chemical engineering, transferring to Brooklyn College for his remaining three years of college. Fortuitously, his academic trajectory was set in his senior year when the professor asked students in a three-person seminar to read Pauling and Wilson, Introduction to Quantum Mechanics, and Mayer and Mayer, Statistical Mechanics. Bob has claimed that he did not understand the texts at the time he first encountered them, although the experience convinced him that he wanted to go to graduate school in chemistry, and specifically to attend the University of Chicago where the excitement and intensity were exactly what he wanted.

During his senior year, Bob became engaged to Susan Sorkin. They had been acquaintances in high school and close friends throughout college, sitting next to each other in classes, sharing books and friends. The story goes that Susan purposefully did poorly in her first chemistry class so that Bob would tutor her in quantum mechanics. The relationship flourished quickly after that, together for the next fifty-one years. They were twenty and twenty-one when they married, when he was still called Bobby by family and friends. To Susan, he was Bobby his entire life.

In his first year at Chicago, Bob decided to be an experimental chemist, joining Clyde Hutchison's research group. He began experiments on the electron paramagnetic resonance (EPR) of a ground state triplet molecule, diphenylmethylene, formed at low temperature by exciting diazo-diphenylmethane with light. Although he managed a successful experiment, obtaining good signals within a few months, he also realized that this was not work at which he would excel. Within the space of a week, he had broken enough large and very expensive dewars to be certain that his skills were not up to the standards either Clyde or he expected. So, he decided to change research groups and become a theorist. Clyde is reported to have claimed that Bob's departure from his group was God's great gift to theoretical chemistry. Working on theoretical chemistry problems with Stuart Rice turned out to be an inspired choice because Stuart allowed his students sufficient freedom to flourish while simultaneously giving them enough advice to make that possible. Stuart suggested a few topics, and connected Bob with Joshua Jortner, a senior visitor in the Rice group, with whom Bob worked on the exciton states of the polyacenes that became his Ph.D. thesis.

After Chicago, Bob won an AFOSR (Air Force Office of Scientific Research) postdoctoral fellowship, choosing to work at the Theoretical Chemistry Institute at the University of Wisconsin. Although he found the work sufficiently challenging to be fun, researching problems in perturbation theory with Joe Hirschfelder convinced him that he wanted to be more connected to novel experiments rather than solely developing theoretical methods.

As he moved from chemical engineering to chemistry, from experimental to theoretical research, and then away from devising analytic methods to explaining experiments, Bob discovered his scientific métier, developing the approach to theoretical physical chemistry for which he would eventually become known and respected: a theorist for experimentalists.

He began as an Assistant Professor of Chemistry at MIT July 1, 1966. Although he joked this was perhaps the lowest paying academic position he was offered, it was the group who gave him the hardest time at his job

talk, so he knew that he would have challenging and exciting colleagues. Once at MIT, he discovered that his colleagues were not only stimulating but unusually supportive and friendly too. Many became life-long friends, sharing a commonsense, pragmatic approach to science as well as academic life, neither too esoteric and removed from ordinary life, nor too consumed by immediate material, government, or corporate interests.

During his early years at MIT, Bob focused on both his undergraduate teaching and graduate student supervision, working on problems having to do with electronic energy transport in solids: exciton energy levels, transport, spectral line-shapes, and phonon scattering. Over the years, he came back to these same issues as experimental techniques improved to provide data about both coherent and incoherent energy transport. It was the second half of the sixties. The Vietnam War was waging; civil rights marches and political protests were routine. Bob showed up at many rallies and teach-ins. He volunteered to teach in experimental programs MIT was developing to address student demands and increasingly diverse interests. At the height of the student protests and antiwar fervor, Bob became the junior faculty resident in Senior House. Both he and Susan organized mini-film festivals and political discussion groups, in addition to Bob's regular tutoring sessions for the dorm residents.

Bob's pedagogic talent was evident from the start. He commanded the classroom with his passion, clarity, and repertoire of humorous stories. A consummate lecturer at the undergraduate and graduate level, he owned the students' attention, mesmerized by the unexpected joy and excitement. He received every MIT teaching award at MIT including the School of Science Teaching Award, the Graduate Student Council Award for Teaching and the Baker Award for Undergraduate Teaching (voted by the undergraduates). In 1996, he was named a Margaret MacVicar Faculty Fellow, an honor that recognizes outstanding classroom teaching at MIT. Together with his colleague Bob Alberty, and later Moungi Bawendi, Bob adapted his lectures for publication in Physical Chemistry, now in its ninth decade of continuous publication, four editions under his authorship.

Throughout his scientific career, Bob kept in close touch with experimental research. He chose theoretical problems that were intimately connected with interesting and important experiments that led to observables easily accessible to measurement. For example, in the area of electronic energy transfer in condensed phases, Bob demonstrated the dominance of quantum effects at low temperatures and was the first to map the change to a classical, incoherent mechanism as the temperature increased.

In the 1980s, Bob recognized that the models used by physicists to explain the newly observed conductivity in doped, but non-metallic polymers such as polyacetylene amounted to Huckel theory, well-known to chemists, with the addition of electronphonon coupling. In short, he provided a physical picture for the origin of the high conductivity as geometric distortions of the chain around the charge, induced by excitations. This work provided the first quantum calculations of the soliton, polaron and bipolaron entities that dominate such polymers' conductivity, essential for polymers' myriad contemporary uses. These polymers have the largest known nonlinear polarizabilities and Bob predicted the saturation of their nonlinear optical properties with chain length, a phenomenon verified in collaboration with MIT synthetic chemists. This work also provided the first quantum method capable of predicting the redox potentials of these polymers, explaining a large amount of existing experimental data in hole burning, photon echo and single molecule spectroscopies, all in agreement with his model and thereby spurring many new experiments.

Bob also worked closely with a global network of experimental chemists and physicists to interpret the optical spectrum of molecules in disordered hosts, in terms of the static and dynamic interactions with their surroundings. He showed that the "two-level system" model for thermal properties of low temperature glasses explained the experimental results of hole burning, photon echo, and single molecule spectroscopy. He went on to use these theoretical ideas for the interpretation of the spectrum of a single quantum dot, and in particular for the spectrum of the light harvesting complex, which is the structure within plant cells that converts light to chemical energy in the process of photosynthesis. He and a colleague showed how quantum friction or noise both slows down and speeds up the energy transfer efficiency within the complex. Developing a wide range of theoretical methods that have now become the standard techniques for studying photosynthetic energy transfer, Bob's work sets the foundation for the new field of quantum biology.

Bob's work was always a collaboration with his more than 65 graduate students and postdocs, for whom he was known as a caring mentor. He challenged them to work on problems of their choosing, yet supported their interests and ingenuity with guidance, insight and encouragement. Acknowledging his role model, many of his students have gone on to positions of leadership in academia. All remember his love of science and his devotion to family and close friends as indivisible parts of his life.

Beginning with the department Head of Chemistry from 1990-1995, Bob took on a series of administrative positions at MIT including the Director of the Center for Material Sciences 1998-2000, and Dean of

Science 2000-2007. Although he never sought leadership positions, and was reluctant at each move to give up teaching, Bob found unexpected pleasure in the new science he was learning as the Dean of Science. He led by example through his own dedication to teaching, research and the success of MIT's students, developing a reputation for extraordinary political acumen. He had the unique ability to work calmly through the most difficult issues, forging agreements from contentious and strong-willed colleagues while bringing people together through humor. With his wit and abundant wisdom, Bob was the obvious person to chair committees whose work required consensus among competing factions. Just since 1998, he was the chair of the Task Force on the Undergraduate Educational Commons, co-chair of the Task Force of Student Life and Learning, co-chair of the Special Faculty Committee on Promotion and Tenure Processes, and member of the Review Board on Campus Police, Faculty Policy Committee and the Skolkovo planning committee. Prior to that, Bob served as the chair of the Institute Calendar Committee, on the Committee on Women Faculty in the School of Science, on the MIT-Wellesley Exchange oversight committee, as an initial developer of Concourse, and was the person who convinced the MIT administration to release the data that lead to the historic report "A Study on the Status of Women Faculty in Science at MIT." An advocate for excellence in teaching, Silbey supported innovative approaches to undergraduate education such as the Technology Enhanced Active Learning program, which changed the way freshman physics is taught.

Bob also made multiple contributions to curriculum innovation. He was a participant in the SP01 experiment and most recently, with chemistry and biological engineering colleagues, he revamped the thermodynamics class, 5.60, that he had taught for many years, making the fundamental principles of energy studies available to students across multiple disciplinary boundaries. He also oversaw the construction of the Brain and Cognitive Sciences Complex and the Physics in-fill building, while beginning plans for the new Center for Cancer Research.

Robert J. Silbey was a fellow of the National Academy of Sciences, the American Academy of Arts and Sciences, the American Association for the Advancement of Science and the American Physical Society. He was awarded the Max Planck Research Award of the Humboldt Foundation, and was a Dreyfus Foundation Teacher Scholar, Sloan Foundation Fellow and a Guggenheim Foundation Fellow. He also received, among other awards, honorary degrees from his alma mater, CUNY Brooklyn College, and École Normale Supérieure in Cachan, France.

After a youth spent perfecting his skill at both chess and pool hall billiards, Bob took up sailing about the same time he began his term as department head. He told Susan that he needed some way to stop thinking about the administrative side of MIT. Sailing the choppy and unpredictable waters of Buzzards Bay from May through October, Bob shared his new-found passion for messing around in boats with his brother-in-law Dick Merians and any students, visiting scientists, or family members, he could shamelessly seduce aboard for a day of boredom punctuated by crisis. During all seasons, Bob listened to jazz and read: the daily papers, the weekly New Yorker, the bi-weekly New York Review of Books, and hundreds of novels and histories. He insisted on completing the crossword puzzle each day before he went to work in his plaid shirt, jeans, and during sailing season without socks. Nearly every picture of Bob is in a plaid shirt and jeans. It is unclear to this day whether he is wearing the same shirt in the pictures or whether his closet is filled with shirts too similar to tell apart. Bob had a style, both sartorial and irreverent.

There was never much separation in Bob's life between work and family and so his family was inescapably a part of his life at MIT. He often used family members as characters in the stories with which he would regale students and colleagues. From early in his career, Susan, and as they arrived Anna and Jessica, were often with him in his office, so much so that like Susan, his colleagues in physical chemistry also called him Bobby. And when the grandchildren, Charlotte, Harper, Henry, and Oliver arrived, he introduced this next generation to life at MIT. He was a caring and loving husband, father, and grandfather who provided unwavering affection and unparalleled wisdom. After spending from 1970 to 1994 raising their young daughters in suburban Newton, Bob and Susan moved back into the city, to their roots as urban youths, no longer hanging out on street corners that had been their meeting ground as teenagers but walking to their favorite sushi restaurant, ice cream parlor, movie theater, the symphony, or Fenway Park. Bob could see MIT from his desk at home and could walk there in 12 minutes. After twenty-four years riding the bus or driving in his mammoth 1973 Chrysler, he returned to the urban life he called home.

In many ways, Bob's life was like the jazz he loved, improvising over a few basic lines. "You don't have to play all the notes," he would often say, paraphrasing Miles Davis. Elegantly understated, he let the silences do much of the work. And Bob Silbey could dance, boy, could he dance...

Agenda

Thursday, December 6, 2012

1:00 ***Welcome:***
Ron Chance and Jean-Luc Brédas, Georgia Tech

Session Chair: Ron Chance

1:15 ***Frank C. Spano, Temple University***
"Novel Mechanisms for Forming J-aggregates, H-aggregates and Those In-Between"

2:00 ***David Beljonne, University of Mons***
"Beyond Förster Resonance Energy Transfer in Biological and Nanoscale Systems"

2:45 ***Rigoberto Hernandez, Georgia Tech***
"Free Energy and Structure in Biomolecular Pulling Simulations"

3:15 ***Coffee Break***

Session Chair: Jean-Luc Brédas

3:45 ***Jérôme Cornil, University of Mons***
"Charge Transport in Organic Semiconductors: From Molecular Junctions to Supramolecular Assemblies"

4:30 ***Veaceslav Coropceanu, Georgia Tech***
"The Effect of Static and Dynamic Disorder on Charge Transport in Organic Molecular Semiconductors"

5:00 ***Demetrio da Silva Filho, University of Brasilia***
"Charge Transport in Organic Semiconductors: Probing High Mobility with Light"

5:30 ***Angelo Bongiorno, Georgia Tech***
"Chemical Structure and Metastability of Graphene Oxide"

Friday, December 7, 2012

Session Chair: Frank C. Spano

8:45 ***Greg Scholes, University of Toronto***
"Lessons From Nature About Solar Light Harvesting: A Little Bit of Coherence?"

9:30 ***Yuan-Chung Cheng, National Taiwan University***
"On Excitonic Phenomena in Molecular Aggregates: A Tribute to Robert J. Silbey"

10:15 ***David Sherrill, Georgia Tech***
"Understanding Non-covalent Interactions in Experimental Systems through Quantum Chemical Analysis"

10:45 ***Coffee Break***

Session Chair: David Beljonne

11:15 ***David Yaron, Carnegie-Mellon University***
"Lowering the Cost of Electronic Structure Calculations by Embedding Empirical Parameters in Ab Initio Theory"

12:00 ***Troy Van Voorhis, Massachusetts Institute of Technology***
"Modeling Organic Semiconductors: It's Silbey's Fault"

12:45 ***Concluding Remarks:***
Ron Chance and Jean-Luc Brédas, Georgia Tech

Frank C. Spano
Department of Chemistry,
Temple University
Philadelphia, PA, USA

"Novel Mechanisms for Forming J-aggregates, H-aggregates and Those In-Between"

The interactions between molecules closely associated in aggregates, films and crystals profoundly impact their electronic and optical properties. Understanding the nature of such interactions is not only of fundamental interest, but aids in the design of more efficient electronic devices such as solar cells and light emitting diodes based on conjugated molecules and polymers. Two extremes in photophysical behavior occur in the conventional J- and H-aggregates, in which through-space interactions determine the ordering of exciton states. In this talk several nonconventional J and H-aggregates will be presented. These include i) charge-transfer mediated J- and H-aggregates in which through-space coupling is negligible, ii) single-chain conjugated polymer "J-aggregates" and their associated HJ-aggregate (π-stacked) hybrids, and lastly iii) carotenoid H-like aggregates in which the nearest-neighbor head-to-tail interactions are J-like. In all such cases the assignments of J-like and H-like are based on vibronic spectral signatures, more reliable than the more conventional spectral shifts.

I have known of Bob Silbey since I first learned what an exciton was. The consummate teacher and scholar, Bob delivered the most stimulating and entertaining talks, usually peppered with good jokes and anecdotes. Humble he was as well, and I recall one occasion – I believe it was at a Gordon Conference – where he stood up at the reception and announced a correction to a Science article he had coauthored. I remembered thinking that the Great One was not only a brilliant scientist but a man of real integrity and honor. Unfortunately, I did not get to know Bob on a more personal level until the last years of his life. One of the greatest honors for me was visiting Bob at MIT and giving a lecture at the Center for Excitonics. Bob was such a gracious and supportive host. I will never forget it.

David Beljonne

Laboratory for Chemistry of Novel Materials, University of Mons
Mons, Belgium

"Beyond Förster Resonance Energy Transfer in Biological and Nanoscale Systems"

After photoexcitation, energy absorbed by a molecule can be transferred efficiently over a distance of up to several tens of angstroms to another molecule by the process of resonance energy transfer, RET. Examples of where RET is observed include natural and artificial antennae for the capture and energy conversion of light, amplification of fluorescence-based sensors, optimization of organic light-emitting diodes, and the measurement of structure in biological systems (FRET). Förster theory has proven to be very successful at estimating the rate of RET in many donor-acceptor systems, but it has also been of interest to discover when this theory does not work. We will review a number of these cases here, highlighting some major contributions from Professor Silbey in the field.

The way I will remember Bob is by a Saturday morning in his office of Dean of Sciences at MIT, where he had brewed fresh coffee while waiting for us (I was accompanied by a young student). That day, he derived FRET theory from scratch, identifying the underneath assumptions that could hide some interesting physics. That a man as busy as him was hosting two Belgian visitors in his office on a Saturday morning and penciled new developments to an old theory in front of our eyes has left me speechless in admiration and respect. We (actually he) worked for a couple of hours in the office and then invited us to a seafood restaurant...

Rigoberto Hernandez

School of Chemistry and Biochemistry,
Georgia Institute of Technology
Atlanta, GA, USA

"Free Energy and Structure in Biomolecular Pulling Simulations"

The behavior and function of proteins necessarily occurs during nonequilibrium conditions such as when a protein unfolds or binds. The need to treat both the dynamics and the high-dimensionality of proteins and their environments presents significant challenges to theoretical or computational methods. Nevertheless, the energetics of an unfolding event can be formally obtained using steered molecular dynamics (SMD) and Jarzynski's inequality but the cost of the calculation increases dramatically with the length of the pathway. An adaptive algorithm has been introduced that allows for this pathway to be nonlinear and staged while reducing the computational cost. The potential of mean force (PMF) obtained for neuropeptide Y (NPY) in water along an unfolding path confirmed that the monomeric form of NPY adopts the pancreatic-polypeptide (PP) fold. Adaptive SMD can also be used to reconstruct the PMF obtained earlier for stretching decaalanine in vacuum at lower computational cost. The PMF for stretching decaalanine in water solvent (using the TIP3P water potential) at 300K has now been obtained using adaptive SMD. Not surprisingly, the stabilization from the water solvent reduces the overall work required to unfold it.

Sadly, I never had the great fortune of working with Bob Silbey directly. In the last few years, with Oppenheim and Keyes, Bob had developed an interest in the steered molecular dynamics method that is the subject of my talk. I had hoped to discuss this work with Bob as part of our recent collaboration with Keyes, but alas the interaction with Bob was cut short. Nevertheless, over the years, I have greatly enjoyed the insight he exhibited in his articles. Equally importantly, I have admired the extent to which he supported his students and colleagues both in terms of sharing his ideas and in promoting their careers. He even served as a mentor to Georgia Tech's rising chemistry department simply because some of his students were here. There is therefore little wonder that his former students and we are celebrating his life!

Jérôme Cornil
Laboratory for Chemistry of Novel Materials, University of Mons
Mons, Belgium

"Charge Transport in Organic Semiconductors : From Molecular Junctions to Supramolecular Assemblies"

Bob Silbey really transported me to new horizons with all our frequent discussions, thus motivating a lot the title of my talk. We worked together on understanding charge transport in organic semiconductors and I will start my talk by reviewing our theoretical advances in this area over the years. Interestingly, the same approaches can also be exploited to model triplet exciton diffusion in organic semiconductors, a topic of current interest as evidenced by the increasingly recognized role of triplets in organic-based devices; some recent results dealing with triplet excitons will be next illustrated. I will conclude by showing recent data on transport in molecular junctions to discuss whether chemists can play there a major role by designing molecules for functional junctions.

You always tend to associate people with famous sentences. There was one for Bob every time he was visiting us in Mons: "It is Belgianing my friend" in reference to our traditionally rainy weather. I have been always impressed by the way Bob could simplify problems to grasp the key ingredients and develop simple models and this is clearly an approach that has driven my research over the years. A few years after my postdoc, Bob knew that I would be in Boston for the MRS meeting; he picked me up one night at my hotel, took me to a good restaurant in town and we spent the evening discussing the two of us about science and life. I will never forget that day where a little Belgian guy felt as someone closely related to such a great person!

Veaceslav Coropceanu
School of Chemistry and Biochemistry,
Georgia Institute of Technology
Atlanta, GA, USA

"The Effect of Static and Dynamic Disorder on Charge Transport in Organic Molecular Semiconductors"

In this contribution, we examine the main factors that define charge transport in organic semiconductors. We have considered two classes of systems: semiconductors based on a single component building block (e.g., oligoacenes) and binary charge-transfer compounds. We use quantum-mechanical approaches to derive the electronic and electron-phonon couplings. The temperature dependence of the charge carrier mobility is studied by treating the electron-phonon interaction as a perturbation (Boltzmann theory), in the static approximation (Kubo formalism) and in the framework of mixed quantum/classical dynamics. The interplay of different electron-phonon mechanisms and static disorder on the temperature dependence of the carrier mobility will be discussed.

I first met Dr. Silbey in 2002 at a Gordon Research Conference. By that time, in collaboration with him, Jean-Marie André, and Jean-Luc Brédas, we published a paper on symmetry anomaly in disubstituted benzenes. My favorite memories of Dr. Silbey stem from the time when we worked on a review paper on charge transfer in organic semiconductors. I was very impressed by his vast knowledge and his ability to explain complex issues using a simple back-of-the-envelope calculation.

Demetrio da Silva Filho
Institute of Physics,
University of Brasilia
Brasilia, Brazil

"Charge Transport in Organic Semiconductors: Probing High Mobility with Light"

Recently, an interesting effect was reported on a dicyanomethylene-substituted thienoquinoid oligomer: a three-orders of magnitude increase in electron mobility upon annealing of the spin-coated film. This increase in charge-carrier mobility was also followed by the appearance of an absorption peak, around 1000 nm, not seen in the solution UV-vis spectrum. These experimental results suggest that the annealing procedure is changing the way these molecules pack and this new order is responsible for the observed change in mobility and absorption spectrum. Here, we investigate this structure-property relationship by means of quantum-chemical calculations. We discuss aggregates of two or more molecules and compute relevant parameters to describe the electron mobility (such as the electronic coupling) and the absorption spectrum in order to rationalize the structure-property relationships observed experimentally. Exploratory TD-DFT calculations indicate that a dimer indeed leads to an excited state around 1000 nm, indicating that intermolecular interactions play an important role in the observed effect.

I met Prof. Silbey on my first visit to MIT, in 2002. Everything at MIT was majestic and formal to me. During the week I spent discussing about charge transport with his PhD student Yuan-Chung, we had one meeting with Prof. Silbey. We got to his office (Dean's office) and I first met his assistant. She was so formal and well dressed that if she had told me she was the Dean I would have believed her. We waited a bit for him. I was surprised when I saw him. He was dressed casual and was very friendly. I told him my mentor in Brazil was Prof. Celso Melo and, right of the bat, he asked me whether he or Celso had more hair left. Y.C. and I tried to show him what we had been doing and he listened patiently. I bet most of what we discussed, that was so fantastic to Y.C. and I, wasn't news to him. But he kindly pretended it was...

Angelo Bongiorno

School of Chemistry and Biochemistry,
Georgia Institute of Technology
Atlanta, GA, USA

"Chemical Structure and Metastability of Graphene Oxide"

Graphene oxide is a material with potential applications in nano-electronics, electromechanical systems, sensors, polymer composites, catalysis, energy storage devices, and optics. Synthesized for the first time in 1855, the molecular structure of this material remains, in spite of the efforts, poorly understood to date. This talk presents a combined density functional theory and X-ray photo-emission spectroscopy study of the structural, chemical, and thermo-stability properties of multilayer graphene oxide obtained from epitaxial graphene films. It is shown, in particular, that the metastability characteristics of this novel form of graphene oxide originate from the presence of C-H species in the structure.

It is well known among the scientific community that Robert J. Silbey was an experimentalist's theorist. His works on energy transfer and nonlinear optical properties of glasses, solids and polymers, and the various theoretical methods he developed contributed to explain a large amount of experimental data and continue to this day to spur many new experiments. His works and approach to science represent a model many theoretical chemists like me will continue to follow for many years to come.

Greg Scholes
Department of Chemistry,
University of Toronto
Toronto, Canada

"Lessons From Nature About Solar Light Harvesting: A Little Bit of Coherence?"

Today, driven by the need for cheap and efficient solar power, we turn to photosynthetic organisms and their light-active supramolecular assemblies for bio-inspiration. In this talk I will explain what we have learned recently about the efficient and robust light-harvesting machinery of natural light-harvesting systems. Two-dimensional electronic spectroscopy experiments reveal the existence of coherence among vibronic levels in the initial response of light-harvesting proteins to femtosecond optical excitation. I will describe these recent experiments that reveal a potential role played by coherence, possibly quantum mechanical in nature, in light harvesting. Biological and chemical examples will be reported. While coherence effects may not profoundly change energy migration efficiencies in large light harvesting antenna systems, they likely influence the underlying distribution of energy trapping times. Understanding and controlling these distributions may provide opportunities for quantum engineering in the design of artificial light-harvesting devices.

There are many things I'll always remember about Bob, such as the way he made complex ideas understandable and how he would enjoy conference presentations through the entire conference, always asking interesting questions. What I'd especially like to highlight is how he spent time to be interested in the work of young researchers--his support and suggestions made, and continue to make, an impact for many of us.

Yuan-Chung Cheng
Department of Chemistry, National Taiwan University
Taipei City, Taiwan (R.O.C.)

"On Excitonic Phenomena in Molecular Aggregates: A Tribute to Robert J. Silbey"

We present a theoretical investigation of coherent excitation energy transfer in molecular aggregates based on a polaronic theory, and demonstrate that energy transfer rate predicted by the theory contains both coherent and incoherent contributions that give rise to interesting dynamical behaviors depending on the temperature and strength of electron-phonon coupling. The analysis allows us to shed light on the mechanisms of energy transfer in molecular systems based on the principles of noise-assisted transport and dynamical localization. Our theory has deep roots in seminal works in the 70s and 80s by Silbey and coworkers, whose keen physical insight and exceptional ability to handle diverse problems still continue to inspire us in this field. We also demonstrate applications to photosynthetic light harvesting and artificial systems, elucidating critical issues such as the effects of quantum coherence, structural disorder, energy landscape, non-equilibrium dynamics, and specific vibrational promoting modes.

I joined Bob's research group in 2000. He was already the Dean then, and was extremely busy. We didn't get to see him often. One morning in 2003, he called me at the Zoo, and wanted to meet me at his office. That was the first time ever he phoned me. I remember vividly that I was having great difficulty in my research at that time. "Oh, no! He's not going to tell me to change program, is he?" I was very nervous when entering his office. Bob told me to take a seat, and took up a plastic bag from his desk. "I'm going to Taiwan. Can you pick out the currency for me?" Then, he showed me a tiny piece of paper, which was a chopstick pack of a local restaurant. He told me he visited Taiwan once in 1998, and the taste of its steamed buns was unforgettable. "You must find out its location, and print out the translation," he said, "so I can revisit the place and have a feast."

David Sherrill

School of Chemistry and Biochemistry,
Georgia Institute of Technology
Atlanta, GA, USA

"Understanding Non-covalent Interactions in Experimental Systems through Quantum Chemical Analysis"

Detailed information about non-covalent interactions is hard to probe by direct experiment. Even carefully-designed model systems in solution often feature unexpected and unwanted competing secondary interactions, while gas-phase studies are complicated by the need for supersonic jet expansions and mass-selection techniques. Theory can provide valuable information through accurate computations on model complexes in precisely-defined geometries. Through such theoretical studies, our group and others have provided a very detailed, fundamental understanding of the physics of pi-pi, CH/pi, S/pi, and other prototype non-covalent interactions in the gas phase. This talk will discuss our recent efforts to connect these findings on small, gas-phase model systems to phenomena governed by non-covalent interactions in more complex systems. Collaborative theoretical/experimental studies on molecular torsion balances as probes of pi-pi and CH/pi interactions (and their substituent effects) will be presented.

I did not get to know Bob Silbey as well as I would have liked. I was an undergraduate at MIT from 1988-1992. Professor Silbey had a reputation in the department for being a brilliant researcher, and I am sorry I did not have an opportunity to take a class from him. I had a few occasions to interact with him after I graduated, and he always struck me as a very straightforward person with whom it was easy to communicate. The quality of his research and his dedication to service will make him remembered as a truly great scientist.

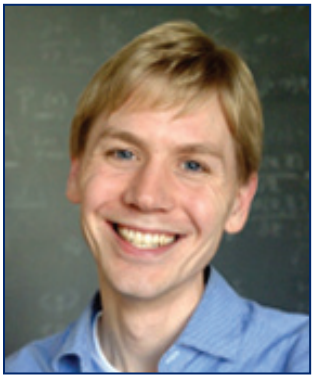
David Yaron

Department of Chemistry, Carnegie Mellon University
Pittsburgh, PA

"Lowering the Cost of Electronic Structure Calculations by Embedding Empirical Parameters in Ab Initio Theory"

Two aspects of molecular structure may be used to reduce the cost of electronic structure calculations. The first is nearsightedness, whereby interactions become simpler at long range. This is the basis for the linear scaling algorithms that are now available for most electronic structure methods. The second is molecular similarity, whereby molecular fragments behave similarly in similar environments. Our goal is to develop a systematic means to take advantage of molecular similarity. Our strategy embeds parameters in a low-level, low-cost, theory and adjust these to obtain agreement with a high-level theory. Such semiempirical parameters can be expected to work over a limited range of molecules. To extend the range of applicability, we make the parameters sensitive to the current molecular context, as captured by the atomic charges and bond orders of the electronic density matrix. Results from the use of this approach on organic molecules will be presented.

Meetings with Bob while I was a post doc were always a highlight of my week. He was a great story teller, whether it was about science or scientists. One of my favorites was about a visit John Deutch made to MIT while he was director of the CIA. John told Bob that he was looking forward to returning to MIT, so that they could team teach physical chemistry, to which Bob responded "over my dead body." John looked at him for a bit and replied, "I think that can be arranged." From my conversations with Bob, I not only learned how to do science, but also learned about science as a human enterprise. He was a great role model for life as a scientist and life among scientists.



Troy Van Voorhis
Department of Chemistry,
Massachusetts Institute of Technology
Cambridge, MA

"Modeling Organic Semiconductors: It's Silbey's Fault"

When I was an assistant professor, I asked Bob for advice about how to build my research program. He advised me to go talk to some of the experimentalists who were doing interesting things and then figure out some theoretical tools that would help them. I followed his advice and ended up being lured into the challenge of understanding electronic processes in organic semiconductors. In this talk I'll review some of the things I've learned from the experiments and some things (I hope) the experimentalists have learned from us as a result of Bob's advice.

Center for Organic Photonics and Electronics
Georgia Institute of Technology
Molecular Science and Engineering Building
901 Atlantic Drive
Atlanta, GA 30332-0400

www.cope.gatech.edu