David A. Kofke of the University at Buffalo

Jeffrey R. Errington, Carl R.F. Lund, and David M. Ford

Dave Kofke pays homage to Boltzmann at Boltzmann's burial site in Vienna.

David A. Kofke displayed an inclination for chemistry at a rather early age. As a toddler he was found inspecting his brother's chemistry set with a bottle of phenolphthalein in hand. Uncertain if he had drunk any, his parents rushed him to the emergency room where they administered the necessary treatment ... ethanol (ethanol inhibits alcohol dehydrogenase from converting the methanol solvent to formaldehyde, which would have made him blind). At the time, his parents were simply happy to recover with a healthy, if somewhat loopy, toddler. Little did they know that this event foreshadowed their son's lifelong commitment to pushing the frontiers of science and engineering. Perhaps it is also this first ominous foray into experimental chemistry that propelled Dave to a career focused on modeling.

Dave was born in Philadelphia and moved to Hempfield, PA, a suburb of Pittsburgh, at the age of one. Dave's brother, W. Andrew Kofke, Professor of Anesthesiology and Critical Care at the Hospital of the University of Pennsylvania, describes a nurturing Kofke household. Their mother, an English-born fever nurse during the Second World War, loved poetry and the works of Shakespeare. She maintained a "high print" household in which books were omnipresent and reading was encouraged. It is their mother that Andrew points to as the one who often promoted the virtues of research. Andrew describes their father as a "handy" guy who was proficient in carpentry and electronics. It was their father who constructed for them custom-made digital alarm clocks well before they were commonplace, and who made Dave a simple knob-operated calculator that he could use to learn his arithmetic tables when he was young.

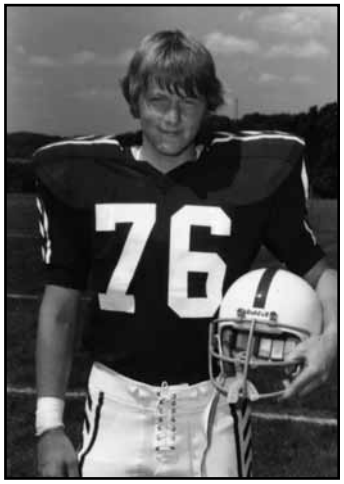
Dave continues in a long line of chemists within the Kofke family. His great uncle, Charles Kofke, received a degree in chemistry from the University of Pennsylvania. His father obtained a B.S. degree in chemistry from Penn State on the GI Bill and spent his career at Gulf Oil. His brother, Andrew, majored in chemistry at Bucknell University before obtaining an M.D. from the University of Pittsburgh. Finally, Andrew's son Matt is defending his doctoral dissertation in chemistry this summer at the University of Pittsburgh. This passion for chemistry made for interesting family events. Andrew conveys stories of their father bringing home pure sodium from the lab and using it to produce "fireworks" on the fourth of July. He also introduced the kids to a paste that exploded upon touch and taught his sons how to make gunpowder.

People who know Dave well often point to his work ethic as a key to his success. This hard-working attitude was shaped at a young age. During his high school years he worked as a "runner" at auctions, and was employed as a sales clerk at Montgomery Ward. In the summer after his freshman year at Carnegie Mellon University (CMU) he worked as a security guard (this is hard for some of us to envision given Dave's generally gentle demeanor). It was during the summers after his sophomore and junior year that he obtained his first technical work experience, at Gulf Oil in Harmarville, PA, as part of their sons-and-daughters program. During his senior year at CMU he received a DuPont Ph.D Fellowship in Chemical Engineering that led to a summer position at DuPont after his senior year. While the experiments he conducted were interesting, it is his interactions with Tammy Gricus that form the lasting memories from this experience ... more on this below.

Dave has always had an inclination for sports. He participated on the high school football team as an offensive lineman. He remains a fan of the game today; he is known to travel to Pittsburgh to catch a Steelers game with his brother or his kids. Sporting activities have also rendered some rather practical discoveries. It was while teaching Dave how to play

Dave and his brother Andrew wait to run Pittsburgh's 10k "Great Race."

School days: Dave in first grade, and as a member of the varsity football team.



baseball that his brother Andrew realized that he was left handed. The skills his brother taught him have been found on display at local softball fields. Whenever the graduate students organize a team, Dave is one of the first to sign up. If you're considering organizing a team, pencil Dave in as your first baseman. Dave's more recent passion is running. He and his brother use their collective interest in running as an opportunity to get together each year to participate in Pittsburgh's 10k "Great Race."

On the education front, there were a number of teachers and experiences that shaped Dave early on. Those of us who are fortunate to work with Dave are familiar with his excellence in writing. For example, Sang Kyu Kwak, Ph.D. 2005, now assistant professor at the Ulsan National Institute of Science and Technology, refers to Dave as a "magician of language." Dave credits his English teacher during his senior year, Mrs. Simmons, as having a profound impact on his development. It was she who gave Dave confidence that he could write well—prior to her influence he saw writing as a chore to be avoided if at all possible. Dave really hit his stride as an undergraduate student at CMU. It was a step change from high school, and in this new environment Dave found he enjoyed meeting the challenges that CMU presented, including those involving writing. In fact, a history professor once tried to persuade him to switch majors, but fortunately for us Dave was not swayed. He found the coursework in chemical engineering, particularly the teaching of Steve Rosen, to be fascinating, and he never doubted his intention to get his degree in chemical engineering.

GRADUATE SCHOOL

Dave arrived at the University of Pennsylvania in the fall of 1983 to start his graduate studies in the Department of Chemical Engineering. Doug Lauffenberger had played a key role in recruiting him, and in fact Dave was planning to work on a project in the bio area. By chance or by destiny, all of the bio projects were oversubscribed, and in looking

The "Glandt ensemble," circa 1985, from left to right, Pat McMahon, Nigel Seaton, Steve Netemeyer, Al Post, Lisa Fanti, and Dave.

around, Dave found that Eduardo Glandt's research program in statistical mechanics piqued his interest.

Eduardo's well-known charisma and sense of humor also played a role in attracting Dave to his group. "I recall meeting with Eduardo to talk about his research," says Dave. "In his usual animated manner he waved his arms and his pen slipped and flew out of his hand and struck him in the neck. Without missing a beat he picked it up and muttered 'What a way to go' while proceeding with his discussion, and I somehow knew then I wanted to work with him."

Dave's Ph.D. research focused on the statistical thermodynamics of polydisperse mixtures, in which the composition is described by a continuous probability distribution over some particle characteristic (*e.g.*, size) rather than a discrete set of species mole fractions. Most notably he proposed the concept of an "infinitely polydisperse" fluid, which has a distribution of chemical potential differences that is logarithmic in the particle descriptor. When particle size is used as the descriptor, the infinitely polydisperse fluid has no characteristic length scale and its thermodynamic properties exhibit a trivial density dependence. Dave also played a role in developing molecular simulations in the semigrand ensemble to study these remarkable fluids. A friend and former groupmate, Nigel Seaton, now principal and vice-chancellor of the University of Albertay, Scotland, remarks that, "Dave's talent for using physical intuition to generate innovative simulation methods to study phase equilibrium was already evident, foreshadowing his important work later in his career. We all knew he was the guy to go to, to check out our thinking on simulation methods."

Nigel also has fond memories of working with Dave on the state-of-the-art computer hardware in the mid-1980s. "One day Dave and I wired up the various, disparate computers in Eduardo's group. We worked it all out, went to Radio Shack to buy the components, and then spent a day doing the wiring. In those days it was a question of opening everything up and connecting the individual wires in the parallel cables to the right pin in the socket. Everything worked, except for one ancient (even in those days) printer. I suppose it wasn't terribly advanced, but a matter of pride for a couple of theoreticians. Nowadays you wouldn't need to, or be allowed to, do that, of course. By the way, this was at about the same time that we upgraded the memory of the group's IBM AT. We ordered, very expensively, 1 Mb of memory, which I seem to remember came in quite a big box, and was a source of wonder and envy to all the other groups in the department." Dave adds that he remembers the boxes of punch cards from Eduardo's thesis work that were idly kept on a high shelf in Dave's office, providing another reminder of how wonderfully modern their own research equipment was.

Those who know Dave today will be surprised to hear that he was not always a master at scientific presentation. Dave calls his first attempt at practicing a presentation in group meeting "pathetically bad" and credits Eduardo and Nigel for teaching him how to speak from a set of slides. Clearly they were successful in their tutelage, as Dave is now known for the clarity and impact of his presentations and seminars.

Penn's Department of Chemical Engineering was (and is) a collegial environment for students and faculty. The accompanying photo shows Eduardo's research group assembling as the "Glandt Ensemble" for a skit at a department party. In the next year they moved from classical to punk, posing as "The Swollen Glandts," for which Dave spiked and dyed his hair. Many lasting friendships and professional relationships were forged. Another friend and former classmate, Steven Weinstein, now professor and head of the Department of Chemical Engineering at the Rochester Institute of Technology, says, "Dave has a great sense of humor that is outwardly contained ... he was always a cordial and great classmate, always unflappable regardless of the pressures of school. He is the kind of guy whose finger you want on the nuclear button." Talk about the ultimate compliment! Eduardo says, "Dave has the unusual combination of being scarily smart and of being impossibly nice. Not surprisingly, he was the most beloved member of the graduate community in the department, since he is such a noble soul. In addition to his big mind and heart, what always strikes me most about Dave is his deliberate style. It's not that he cannot be spontaneous or speak 'stream of consciousness' but one gets the feeling

Fellow Carnegie Mellon alums Dave and his wife Tammy only met when both were working summer jobs at the DuPont Experimental Station in Wilmington, DE.

that in most cases he has mused in advance about what he is saying or writing. I was stunned when he once told me that he sometimes would set time aside ... to think! Who else does that? That's how he discovered some profound concepts, like infinitely polydisperse fluids. He was a totally self-starting student, who initiated most projects himself."

These remarks regarding Dave's humble nature and remarkable dry wit are commonplace when discussing Dave with his friends and family. His brother, Andrew, notes the comic relief he provides during the 10k "Great Race" that they participate in, this past year drawing analogies between the manner in which runners segregate into groups as the race proceeds and the manner in which a fluid mixture separates within a chromatographic column. Donald Visco, a 1999 Ph.D. graduate from Dave's group, now the Associate Dean for Undergraduate Studies within the College of Engineering at The University of Akron, recalls the following interaction with Dave, "I was walking with Dave to a meeting somewhere on campus. I must have been confused or exasperated by something in thermodynamics because I asked him, 'When did you finally understand thermodynamics?' Without missing a beat, he deadpanned, 'I'll let you know when I do.' I chuckled, but I took comfort in the fact that someone as brilliant as Dave, someone who I thought (and still think) was one of the smartest people I know, would allow me to hear such an answer. It made a big impact on me at the time and let me know that my struggle was actually a journey."

Dave started a post-doctoral position with Martin Yarmush at Rutgers in 1988. He wanted to stay close to Philadelphia as his wife, Tammy, finished up her Ph.D. at Penn with Ray Gorte, and perhaps also to indulge his original interest in bio-oriented research. He was at Rutgers for a year and contributed to a paper on energy conservation in the molecular dynamics simulation of proteins. During this time, Dave was offered a National Research Service Award (NRSA) post-doctoral grant from the National Institutes of Health (NIH), but he had to decline as he had accepted a faculty position at the State University of New York at Buffalo.

FAMILY LIFE

Despite growing up near the same city, having attended the same university (Carnegie Mellon) and having the same major (although in different years), Dave did not meet Tammy in Pittsburgh. Instead it was in the summer of 1983, after Dave was graduated and both were working summer jobs at the DuPont Experimental Station in Wilmington, DE. It is that odd effect where perfect strangers from the same town can feel like old friends when they happen to meet somewhere far away from home. Their friendship blossomed into romance during their graduate-school years as Tammy joined Dave at Penn, and they were married in October 1987. Looking back, they realized that as an undergraduate teaching assistant at CMU, Dave had graded Tammy's thermodynamics homework (they still have them), and that in one semester they had taken the same elective course: Genetics!

Like many couples in similar fields, Dave and Tammy faced the "two-body problem" when they sought employment. As Dave started his academic career at the University at Buffalo, Tammy was employed as a Research Engineer at Occidental Chemical's Technology Center in nearby Grand Island, NY. Outside of work in the early years of marriage, Dave and Tammy enjoyed travelling on Tammy's frequent-flyer points. To indulge his inner experimentalist, Dave took up home remodeling as something of a hobby, and made many improvements to their house (wiring projects being his favorite). During this time, Dave also discovered a passion for woodworking. He embarked on many projects for the house and garden, including the construction of a very large picnic table that was used in later years for seating for all the graduate students in Dave's group. To Tammy's dismay, however, most of the projects ended up being fancy tables and stands needed to house the growing collection of woodworking tools. Alas, before Dave managed to build that showcase dining room set, his time became much less elastic. The year 1994 brought two momentous events: Dave received tenure at UB, and his son Alex was born. Three years later daughter Jocelyn arrived. With the combined demands of an academic career and fatherhood, Dave's handyman hobbies have taken a back seat for a while.

UNIVERSITY AT BUFFALO

Dave started at the University at Buffalo (UB) in the Fall of 1989. His academic career got off to a rapid start with a series of early accomplishments. Before arriving at UB he secured a Research Initiation Grant from the National Science Foundation (NSF). In his first year at UB he received a Presidential Young Investigator award from the NSF. These awards jump-started Dave's research program, which is focused on the development and implementation of molecular simula-

"He is the kind of guy whose finger you want on the nuclear button."

—friend and former classmate Steven Weinstein

tion tools for the prediction of thermophysical properties and understanding the behaviors of complex systems. These awards also marked the beginning of a long and productive relationship with the National Science Foundation, as Dave continues to be supported by this organization.

Dave is perhaps best known for development of "Gibbs-Duhem integration," a technique for tracing phase coexistence lines of model systems. At the time the method was introduced, very few techniques existed for locating phase coexistence points, and those available were not suitable for working with condensed ordered phases (*e.g.*, crystalline solids, liquid crystals). The Gibbs-Duhem technique was designed in a way that avoided a key Monte Carlo move that rendered alternative methods ineffective. The new approach was quickly employed by numerous investigators, including Dave and his students, to tackle problems previously deemed intractable. Dave developed the initial ideas for this approach during a month spent as a visiting researcher at the FOM Institute for Atomic and Molecular Physics located in The Netherlands, where he was hosted by Daan Frenkel, a prominent member of the molecular simulation community and now a professor within the Department of Chemistry, Trinity College, University of Cambridge. When reflecting upon the time he spent with Dave at FOM, Frenkel writes, "In 1991, when I invited Dave to spend some time at FOM, I had never met him in person. I had read his papers on the semi-grand ensemble and on chemical equilibria in multicomponent fluids. It was just amazing work: very creative, very clear. I wanted to meet this person. Dave stayed for just under a month in May/June 1992. We discussed many topics, but time was too short to start on any specific project. Only a few months later, Dave sent me a preprint on his Gibbs-Duhem work. Again, a very elegant idea—we later used this method, but I was not involved in the creation. A few years later, my then-student Peter Bolhuis spent a few months with Dave at Buffalo. This visit was a great success. Dave wrote: 'Peter's productivity is exceptional, but the real satisfaction I had from his stay was the regular opportunity to discuss research with him.' Together, they wrote a seminal paper on the freezing of polydisperse hard-sphere systems. I consider it a privilege to be able call Dave not just a (greatly admired) colleague but also a personal friend." Frenkel's comments regarding the creativity, clarity, and elegance of Dave's work are frequently echoed by his peers.

Many of Dave's current research activities grew out of a sabbatical leave spent at the University of Tennessee, where he was hosted by Peter Cummings, now the John R. Hall Professor of Chemical Engineering in the Department of Chemical and Biomolecular Engineering at Vanderbilt University. As chemical engineers can appreciate, the free-energy surface of a system plays an important role in dictating the behavior it exhibits. As a result, molecular simulation is often used to compute various free energies. During his sabbatical, Dave initiated an effort aimed at obtaining a better understanding of the relative accuracy, precision, and limitations of methods used to compute free energy information. The outcome of this work was a series of seminal papers in which he and his coworkers brought clarity to this important issue by outlining metrics that one can use to ascertain the accuracy and precision of various free energy methods. They showed that some methods were fundamentally flawed, while others were robust. Dave is now recognized as one of a handful of people who truly understand the intricacies of free energy calculations. Reflecting upon the time that Dave spent at the University of Tennessee, Peter Cummings writes, "I remember Dave's sabbatical with me as one during which I learned a great deal from him about the subtleties of free energy methods. I had known Dave since he was a graduate student at Penn, and had always admired his insight and originality, and I truly enjoyed the opportunity to interact with him for an extended period on a daily basis. It was during this time that we also wrote a successful proposal to develop a web-based textbook for molecular simulation, using web constructs that were way ahead of their time. Etomica was initiated during this period, as the methodology for producing illustrative simulation applets for the web-based text. All in all, it was a very productive time for Dave and for me."

More recently, Dave and his students are working on the development of computer simulation methods to compute so-called cluster integrals. These calculations provide a means to obtain the virial coefficients necessary for implementation of the virial equation of state (VEOS). Leveraging their knowledge regarding free energy calculations, Dave's group developed a novel formalism for computing cluster integrals. Their advancements in this area have transformed the utility of the overall VEOS approach and have reenergized the prospects of using the VEOS as a practical engineering tool for describing the thermodynamic properties of fluids. Moreover, these developments have enabled the community to better understand various fundamental aspects of virial coefficients.

The direction of Dave's research endeavors often follows the path less traveled. This approach, however, has not hindered his peers from noticing the high quality of his contributions. Now with nearly 120 refereed journal publications, the impact of Dave's work is conveyed by a long list of awards, including the Presidential Young Investigator Award, the Dow Outstanding New Faculty Award of the ASEE, the John M. Prausnitz Award in Applied Chemical Thermodynamics, and the Jacob F. Schoellkopf Medal. At UB and within the SUNY

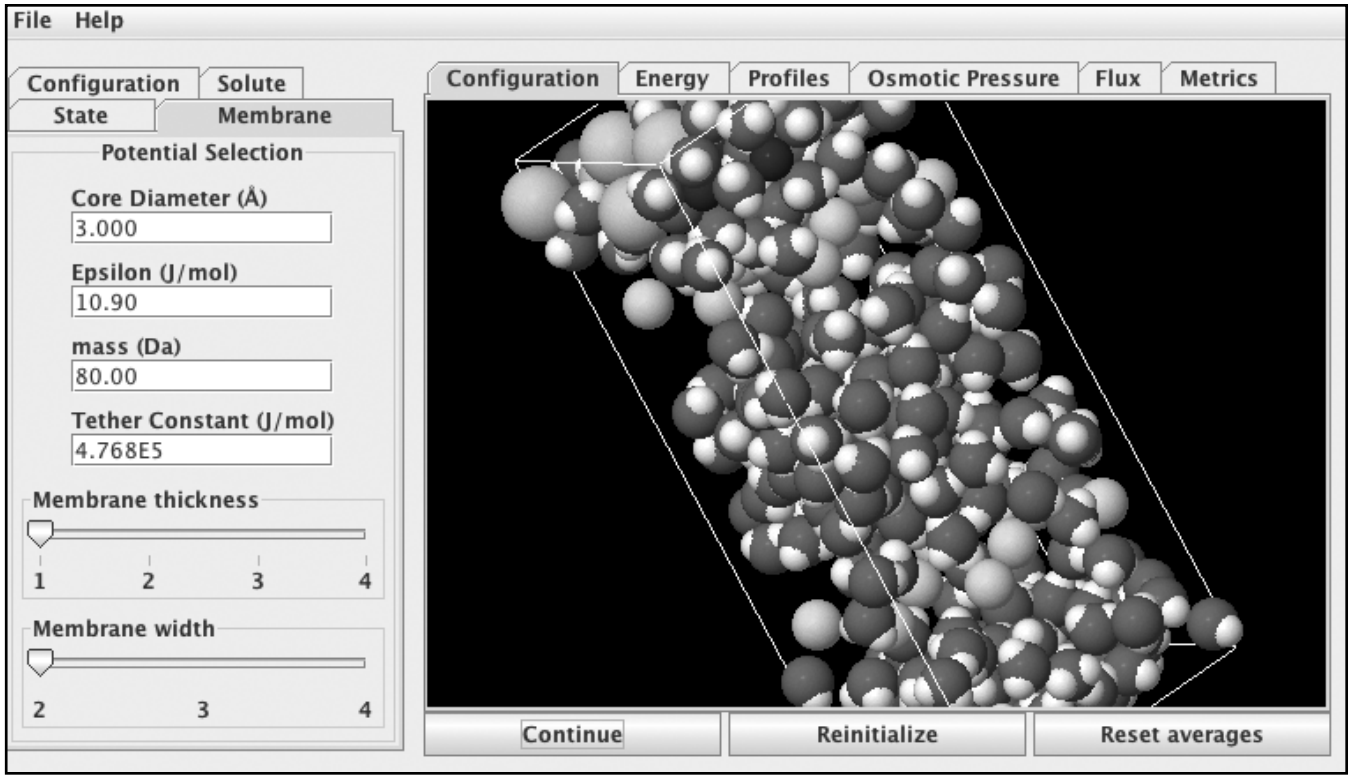
system he has been recognized by the UB Exceptional Scholar Award and the SUNY Chancellor's Award for Excellence in Research and Creative Activity.

TEACHING

Dave is an accomplished teacher, as recognized in 1994 by his selection for the SUNY Chancellor's Award for Excellence in Teaching. His teaching portfolio includes a range of courses that extends from introductory level (introduction to engineering, engineering computations) through chemical engineering core topics (mass and energy balances; fluid mechanics; thermodynamics; unit ops lab) to advanced undergraduate, honors and graduate topics (molecular simulation, molecular modeling, advanced chemical engineering thermodynamics, and statistical mechanics). He is recognized as an excellent teacher by students at all levels.

Professor Kofke's classroom teaching style is largely conventional, at least on the surface. When asked what makes his teaching special, former students point to his mastery of the subject matter, the clarity with which he explains difficult concepts, his ability to make analogies to everyday life, his ability to see course material from the students' perspective, the quality of his homework and exam questions as teaching/learning vehicles, his preparation for class and organization, and his mentoring skills. Of all the positive qualities they mention, however, the one that comes through most consistently and strongly is the amount of time he makes available to the students in his classes. David Ford, who did undergraduate research with Dave, went on to obtain a Ph.D. in statistical thermodynamics and now is a professor himself at the University of Massachusetts recalls one example, "One lasting memory I have is going to see Dave for help with a homework problem from the fluids class that I was taking from another instructor. I was looking for the fluids instructor, but he wasn't in, and I happened to see that Dave was in his office so I asked him. It turned out that the solution wasn't obvious to Dave either, but he spent at least half an hour thinking through it with me and searching though his transport books. We finally found the answer in an example in Perry's *Chemical Engineer's Handbook*, of all places. Only later, when I became a faculty member and experienced the many pressures and time constraints on an assistant professor, did I truly appreciate Dave's generosity in helping me that day."

Dave recognized the important role that computer technology could play in education early in his career. One of his early educational technology projects was a simulator for teaching chemical engineering concepts. From those beginnings, Dave led the development of etomica, an open-source library that can be used to construct molecular simulations using JAVA. Recognizing that molecular simulation could be applied to teaching in a very wide range of subject areas, Dave was instrumental in the creation of the etomica modules



Snapshot of the Osmosis molecular simulation module.

Group party at the Kofke home in 2003. Back row (left to right): Chris Iacovella, Jayant Singh, Sang Kyu Kwak, Scott Wierzchowski, Dave, Jhumpa Adhikari. Front row: Children Jocelyn and Alex, Nancy Cribbin, Di Wu.

(<modules.etomica.org>). With funding from NSF, through CACHE, a process was devised whereby experts from a given field could propose the creation of a molecular simulation module. Twelve simulation modules were created via collaboration with the experts who had proposed them. These experts produced the documentation for the modules with examples and problems that used them. Working closely with Andrew Schultz, Dave created many additional modules of his own device and included them in the etomica modules. The educational effectiveness of the modules was established through an independent assessment conducted at more than 10 institutions. The modules now receive more than 4,000 hits per month, not counting internal access and search engine web crawlers.

The etomica modules now enjoy widespread use. Dave has conducted molecular simulation workshops at the ASEE Chemical Engineering Summer School and at FOMMS (Foundations of Molecular Modeling and Simulation) Meetings. Dave has also collaborated with the Center for Computational Research at UB in hosting workshops on molecular simulation for high school students. Peter Cummings notes that etomica "has become THE tool for introducing molecular concepts to students (*e.g.*, answering, with visualization and virtual experiments, what is the molecular basis for diffusion? for viscosity? for phase equilibria? of the Joule-Thompson effect?, of pressure?, etc)," and he points out that "... we always find that it is the quickest way for a neophyte to obtain a hands-on idea of what molecular simulation is all about. Etomica modules can be used in any course by any instructor wanting students to learn about the molecular basis for a particular phenomenon."

Professor Kofke's service contributions to the profession and to his department also have been significant. Upon his arrival at UB, he became a member of the department's Undergraduate Committee, and within two years he became its chair. He created the department's first website and has

been active in its expansion and evolution ever since. He guided the department through a significant curriculum revision during that time, as well. His philosophy is reflected in a colleague's recollection of Dave's participation on a different school-wide teaching oversight committee. In light of concerns over student retention and graduation rates, the committee had drifted into a discussion of ways to change one particular course so students would struggle less to pass it. Dave quickly pointed out that the focus needed to be placed on better ways to teach the more difficult material, not on reducing the rigor of the course. As such, it perhaps is not surprising that Dave implemented a web-based platform for departmental curriculum evaluation and assessment. It has served as a model for other departments in the School of Engineering and Applied Science.

Dave was a founding member of an ad hoc committee for high-performance computing that led to the creation of the Center for Computational Research at the University at Buffalo. He has served as chair of its Scientific Board since 1999. He is currently nearing the end of his second term as the chairperson of the Chemical and Biological Engineering Department (which for the past two years has coincided with his co-chairing of a new Biomedical Engineering department at UB). His tenure has been characterized by an increase in the number of faculty, planning a 33% expansion of the Department's space, creation and endowment of a symposium series that honors Eli Ruckenstein, rejuvenation of the Department's advisory board, and continuation of a department atmosphere that is open to comment, suggestion, and debate.

Notable among his other professional service activities, Professor Kofke was elected a trustee of CACHE in 1999. He served as its secretary from 2004 to 2006, vice-president from 2008 to 2010, and is now completing a two-year term as its president. Dave has been an active member of CACHE's Task Force on Molecular Modeling since 1996. He is a member of the AIChE, ACS, and AAAS, and has served as an AIChE Area 1a programming chair. He has been a member of the editorial board of *Molecular Physics* since 2007.

MENTORSHIP

David Kofke has mentored more than 20 Ph.D. students, 10 M.S. students, and countless undergraduates. Discussions with his former students paint a picture of a man who is influential, inspirational, intelligent, patient, respectful, ambitious, and of high integrity. Donald Visco writes, "Dave Kofke was the most influential person in my academic career. He was incredibly patient, treated everyone with respect, and was a tremendous role model for someone who wanted to obtain a faculty position, like me. In fact, he still is a great mentor and I continue to seek his counsel on a variety of items." From Jayant Singh, Ph.D. 2005, now an associate professor within the Department of Chemical Engineering at IIT Kanpur, "Dave has been inspirational for me, as a teacher, guide, and human being. I remember clearly coming to UB to work with Prof. Ruckenstein. However, after talking to Dave and seeing his eyes fill with zeal, I immediately decided to work with him. ... As I have got to know Dave more, my admiration and respect have grown exponentially. Such a wonderful teacher and guide who allows one to grow in person and academically is difficult to find. I have been lucky and blessed to be associated with Dave and I know that it is difficult to walk on his footstep." Sang Kyu Kwak adds, "He made the greatest and most delightful impact on my life, which I will cherish as long as I live."

As noted above, Dave is known for his humble nature. As Durgesh Vaidya, Ph.D. 1997, now senior manager of Research and Development at OFS, points out, this should not be associated with a lack of ambition, "Most people surmise Dave to be brilliant, yet soft-spoken and easy-going. Those that work closely with him will recognize that, like all good leaders, he is ambitious—not for himself but for his cause. I once recall working very hard over several weeks to come up with something that was about 20-25% better than the best of the previously published record. When I discussed this with Dave, he listened patiently and then remarked, 'Good idea, yet it is incremental research. We are here to do radical research. That's where the real fun is!' By the time our project was over, we had found a way to improve it by an order of magnitude." While Dave encourages his students to strive for greatness, he reminds them that integrity matters. Again from Durgesh Vaidya, "One day Dave came to our workstations with photocopies of a letter someone had written to a well-known journal. The letter was a rather harsh criticism of a previously published research article, in which the authors had made a small error that rendered their claims of significant achievements flawed. Dave quietly remarked to all in his group, 'Remember, please make sure your work is correct first. We will worry if it is interesting later.' I have never forgotten those words."

Dave and Tammy regularly host dinners for the group. Many of his students have lasting memories of these social gatherings. Scott Wierzchowski, Ph.D. 2003, now a research engineer with Shell, writes, "I remember all the times he would have us to his house for the holidays and parties. It sure made our group feel like a little family. It was very genuine and appreciative." Jhumpa Adhikari, Ph.D. 2003, now an associate professor within the Department Of Chemical Engineering at IIT Bombay, adds, "... as an international student I especially enjoyed the group visit to his home where one of my oft-recounted stories is of the decorated Christmas tree that I saw for the first time in a family setting, about which I had only read in books before."

One of the authors of this article (JRE) has also benefited tremendously from Dave's mentorship. As an undergraduate student at UB, he introduced me to the field of molecular modeling and guided me towards the profession I enjoy today.

At the time, I was fairly ignorant about graduate school and had questions like 'do you get to go home over the summer?' and 'is it worth taking on additional student loans?' He took me under his wing and helped clarify what now seem like trivial issues and provided confidence that graduate school was appropriate for me. He also alerted me to more significant issues, like the importance of identifying an advisor and institution that provide the right environment for success. It is this experience that often motivates me now to make the extra effort with our undergraduates. In my current position as a faculty member at UB I continue to seek his advice, support, and, at times, motivation. For me, Dave is the ideal mentor. His advice is direct, but never dogmatic, and the motivation for his comments is never derived from his own self-interests. I also appreciate how he leads by example, always pushing for excellence in research, teaching, and service. His high standards, self-sacrificing nature, attention to detail, and positive attitude make those around him better. I often find motivation to improve by benchmarking my professional progress against Dave's trajectory. It's a hard act to follow!

AWAY FROM THE OFFICE

These days much of Dave's life away from the office revolves around his family's activities. Alex is now finishing his senior year in high school, and Jocelyn is a freshman. Music has a very strong presence in their home, as Alex has developed into an accomplished oboist, and has shown a strong natural ability with other instruments (he performed a movement from a Rachmaninoff piano concerto for his senior concerto, after only two years learning the instrument). He also has a strong passion for classical music in general, and Dave and Tammy's appreciation for this genre has grown enormously just by being around him. After seriously considering going to college as a music performance major, Alex examined the career options in this direction and decided to pursue physics instead, perhaps with a minor in piano. Jocelyn's instrument is the baritone saxophone. She is still unsure of her career path; she inclines toward art, but excels in all her courses. Dave has found a connection with her through their mutual enjoyment of softball, as well as some traveling adventures (most recently to New York City, and with a trip to Paris in the works now). Family vacations usually entail a week in the Adirondacks.

When not with the family, Dave participates in a philosophy-oriented book club that meets monthly; also, over the past 10 years he's taught himself piano—he particularly likes playing Bach, but is definitely not at a performance-ready level. In slightly less cerebral pursuits, he enjoys watching both recent and classic movies. He built a home theater to enhance this activity, but anymore he's happy if he is just able to stay awake through the whole show. And as much as he likes music, most often he prefers the calming white noise provided by a good fan. His favorite is the vintage Vornado that was built in the 1950s, and that was a constant presence in his childhood (he's amassed quite a collection of them, thanks to eBay). And while this and the many other factors recounted above have made Dave what he is today, fortunately, one childhood influence he did not carry into adulthood is any taste for phenolphthalein! ❐