Y. Apeloig

*Y. Apeloig has recently published his **10th article** since 2000 in Angewandte Chemie*:
"Radical Polymerization of the Silene $(Me_3Si)_2Si{=}CR_2$ by Hydrogen Transfer from a Trimethylsilyl Group": D. Bravo-Zhivotovskii, S. Melamed, V. Molev, N. Sigal, B. Tumanskii, M. Botoshansky, G. Molev, Y. Apeloig, *Angew. Chem.* **2009**, *121*, 1866–1869; *Angew. Chem. Int. Ed.* **2009**, *48*, 1834–1837.

Yitzhak Apeloig

Date of birth:	September 1, 1944
Position:	Professor of Chemistry and President of the Technion–Israel Institute of Technology, Haifa
Education:	1962 High School diploma, Ramat Gan (Israel) 1964–1967 BSc degree, Hebrew University of Jerusalem (Israel) 1967–1969 MSc degree, Hebrew University of Jerusalem 1969–1974 PhD with Z. Rappoport, "Intermediates in S_N1 Vinylic Substitution", Hebrew University of Jerusalem 1974–1976 Postdoc with P. von R. Schleyer, Princeton University (USA) in collaboration with J. A. Pople, Carnegie–Mellon University (USA) 1983–1984 Sabbatical with R. Hoffmann, Cornell University (USA)
Major awards:	**1991** and **1999** Japan Society for the Promotion of Science Award (JSPS); **1994** Alexander von Humboldt Senior Research Award; **2002** The Israel Chemical Society Prize; **2006** Honorary Doctorate from The Technical University of Berlin, (Germany); **2007** Wacker Silicone Award (Germany)
Current research interests:	1) Organosilicon chemistry with emphasis on low-coordination silicon compounds, such as multiply-bonded silicon compounds, silyl radicals, anions and silylenes, as well as the development of new silyl–lithium and other metallosilane reagents. 2) Computational chemistry, emphasizing the interplay between theory and experiment. 3) Physical organic chemistry including, aromaticity, strained molecules, reactive intermediates, and reaction mechanisms
Hobbies:	Traveling, music, skiing, and history

My favorite subject at school was … soccer.

When I was eighteen I wanted to be … a scientist.

When I wake up I … rush to prepare coffee!

The most significant scientific advance of the last 100 years has been … the communication revolution—from the telegraph and the telephone to the cell phone and the internet.

The biggest challenge facing scientists is … explaining what we do to the public and the decision makers.

My favorite piece of research is … the Woodward–Hoffmann orbital symmetry rules and related experiments.

If I could have dinner with three famous scientists from history, they would be … Albert Einstein, Louis Pasteur, and Marie Curie.

I chose chemistry as a career because … everything around us, including ourselves, is chemistry!

My first experiment was … preparing propellants for a home-made toy rocket!

If I wasn't a scientist, I would be … an archeologist.

My biggest motivation is … to educate a new generation of scientists.

In my spare time I … love traveling and discovering new cultures, and also listening to music.

The secret of being a successful scientist is … originality and hard work.

I would have liked to have discovered … penicillin and oxygen

The most groundbreaking discovery in science in the past 100 years has been … It is impossible to say—there are hundreds of discoveries that have transformed the world!

My favorite musicians/composers are … Beethoven, Mozart, and Mahler.

The most significant advance in chemistry of this century has been … the development of new analytical and separation methods and tools.

The biggest challenge facing chemists is … as it has always been—deciphering the secrets of nature and using this knowledge to benefit humanity with an emphasis on sustainability and the environment.

How is chemistry research different now than it was at the beginning of your career?

The "computer revolution" had a major impact on my research. When I was working on my PhD, computers were too slow to allow their useful application to chemistry (certainly organic chemistry). Since then, the speed and power of computers has increased by a factor of 10^7–10^8, making it possible to use theory (in particular quantum-mechanics) to make reliable predictions for a variety of physical and chemical properties (including reactivity) of compounds, including large biological molecules. The dream of "first calculate then synthesize" has become a reality!

In the experimental arena, the development of NMR spectroscopy, X-ray diffraction, and mass spectrometry has been amazing, allowing chemists to make advances that we did not even dream of 40 years ago!

Has your approach to chemistry research changed since the start of your career?

As stated above, the motto of "first calculate then go to the laboratory and synthesize", which was not possible 40 years ago, now leads our way in many of our studies. Quantum-mechanical calculations have reached a level of high reliability, allowing us to predict which molecules can exist and their lifespan under certain conditions. Consequently, we routinely use calculations to guide our search for novel types of molecules. The dream of quantum chemists, after the Schrödinger equation was published, to apply quantum mechanics to chemistry and biology is becoming a reality, certainly for medium-sized molecules.

Has your approach to publishing your results changed since the start of your career?

Not much. As others, I aim to publish in the best journals with refereeing procedures that can be trusted. Publishing in first-rate journals is especially important for the future career of our students. Throughout my career I have always been amazed by the vast amount of work that referees have put into reviewing my papers (and I do the same for others, of course) and have found that in most cases their comments and inputs have significantly improved our work and the article. This is an opportunity to thank all of these anonymous referees.

What do you think the future holds for your field of research?

My research interests are in two fields: computational chemistry and organosilicon chemistry. Computational chemistry has undergone a vast revolution. Yet, I see rapid progress also in the future, both in computer technology and even more so in the development of new computational methods. In the foreseeable future, we will be able to reliably treat very large molecules, solvation effects, and many other important chemical phenomena. Chemists and biologists will routinely use computations in their work.

Silicon chemistry has also undergone a revolution. Many molecules, which only 40 years ago were believed to be incapable of existence, have been synthesized and isolated, but the field is still in its infancy. In the future, an entire range of low-coordination silicon compounds will be discovered and explored, and we will see practical applications of these novel compounds as, for example, precursors to new types of silicon-based polymers. The field of synthetic organosilicon chemistry is also in its infancy and the future will bring new reagents and synthetic methods, which will expand the current limited arsenal of synthetic tools, opening up many new opportunities. Bio-organosilicon chemistry is yet another important and poorly explored frontier. The future should also bring a deeper understanding of the fundamental question "why do silicon and carbon compounds behave so differently although they are 'close relatives' in the Periodic Table?", which is a question that is also relevant to other main-group elements.

I have always been amazed by the vast amount of work that referees have put into reviewing my papers ... In most cases their comments and inputs have significantly improved our work and the article.

Have you changed the main focus of your research throughout your career and if so why?

Yes, several times. My PhD research (with Z. Rappaport, Jerusalem) was in classical mechanistic organic chemistry (solvolysis of vinyl derivatives). During my postdoctoral studies (with P. von R Schleyer and J. A. Pople), I was introduced to computational quantum chemistry and I was immediately fascinated by its vast potential, although at that time (1974) this new discipline was met with great skepticism (and was even ridiculed) by most experimental chemists as being irrelevant to their research. Upon returning to Israel, I combined computational chemistry with experimental studies in physical organic chemistry (carbocations, hyperconjugation). In the 1980s I was attracted to low-coordination silicon chemistry, in particular, I was amazed by the vast contrast between silicon and

carbon compounds such as the non-existence of most Si=X compounds. A combination of theory and experiment appeared to be the best way to proceed in this unexplored territory, and this synergism indeed proved to be extremely beneficial, leading to many discoveries.

What has been your biggest influence/motivation?

My biggest motivation was the drive to understand nature and to be able to manipulate it to the benefit of humanity. This fascination with chemistry is responsible for the fact that I continue to be actively involved in research, despite many obligations during my eight-year term as president of the Technion–Israel Institute of Technology.

The largest influence has been that of my wonderful teachers, especially my supervisors during my PhD and postdoctoral studies.

What advice would you give to up-and-coming scientists?

"Follow your heart" and study what excites you. Choose an important scientific question to which you believe you can make a significant contribution and be patient—progress in research is usually very slow!

What is the secret to publishing so many high-quality papers?

The "secret" is in having an excellent and dedicated research group with students and co-workers who think independently and have original ideas. In my own case, the fact that I could continue publishing high-quality papers during my term as president of the Technion is certainly first and foremost an accomplishment of my outstanding research group.

My 5 top papers:

1. "Substituent Effects on the Carbon–Silicon Double Bond. Monosubstituted Silenes": Y. Apeloig, M. Karni, *J. Am. Chem. Soc.* **1984**, *106*, 6676 – 6682.
   In this paper we used theoretical calculations to predict the substituent effects on the stability of silenes (R_2C=SiR_2) to show, for example, that silyl substitution on the silicon atom reduces the inherent polarity of silenes and dramatically increases their kinetic stability. This insight, which was gained from theory, guided our experimental work (as well as the work of other experimental groups) and lead to the synthesis of novel silenes (e.g., see reference [3] below). This paper was also important in demonstrating to many skeptical experimentalists in the field just how important calculations can be in directing experimental efforts to synthesize unknown compounds.
2. "A Theoretical Survey of Unsaturated or Multiply Bonded and Divalent Silicon Compounds. Comparison with Carbon Analogues": B. T. Luke, J. A. Pople, M. B. Krogh-Jespersen, Y. Apeloig, M. Karni, J. Chandrasekhar, P. von R. Schleyer, *J. Am. Chem. Soc.* **1986**, *108*, 270 – 284.
   Here we used theory to systematically predict the structures and energies of all possible combinations of two heavy-atom (Li to F) unsaturated or multiply-bonded silicon compounds and compared them with their carbon analogues. The level of theory that could be applied at that time was quite simple (3-21G*), yet we believed in its reliability and took a risk in challenging experimentalists to follow and test the predictions. Eventually, this study served as a guide to many experimentalists (both gas-phase and solution chemists) in their search for new silicon compounds. This study was a clear demonstration to many skeptical experimentalists of the power and the reliability of quantum-mechanical calculations as a guide for experiments.
3. "Novel Route to Carbon–Silicon Double Bonds via a Peterson-Type Reaction": D. Bravo-Zhivotovskii, V. Braude, A. Stanger, M. Kapon, Y. Apeloig, *Organometallics* **1992**, *11*, 2326 – 2328.
   Following the theoretical insights gained in reference [1] above, we developed a novel method (sila-olefination) for the synthesis of C=Si bonds. This lead to the synthesis and isolation of several new silenes, including the first metal-substituted bis-silene (see reference [5] below). The synergism between theory and experiment was excellent.
4. "HCSiF and HCSiCl: The First Detection of Molecules with Si≡C Triple Bonds": M. Karni, Y. Apeloig, D. Schröder, W. Zummack, R. Rabezzana, H. Schwarz, *Angew. Chem.* **1999**, *111*, 343 – 347; *Angew. Chem. Int. Ed.* **1999**, *38*, 331 – 335.
   The synthesis of compounds that form triple bonds to silicon was (and still is) one of the "Holy Grails" of silicon chemistry. We approached this demanding challenge by a combination of theory and experiment. Calculations were used to analyze the problem, leading to the design of a sophisticated gas-phase experiment (carried out by the group of H. Schwarz, Berlin), which for the first time, detected the triply-bonded silyne. This demonstrated that the theoretical strategy is valid, paving the way in the future to the synthesis, and hopefully isolation, of other silynes.
5. "The Synthesis and Isolation of A Metal Substituted Bis-silene": D. Bravo-Zhivotovskii, R. Dobrovetsky, D. Nemirovsky, V. Molev, M. Bendikov, G. Molev, M. Botashansky, Y. Apeloig, *Angew. Chem.* **2008**, *120*, 4415 – 4417; *Angew. Chem. Int. Ed.* **2008**, *47*, 4343 – 4345.
   In this paper we used the methodology and the new metallosilane reagents that we have developed over the last decade to synthesize and isolate the first bis-silene with two C=Si bonds. Furthermore, the two C=Si bonds are connected through a metal (Hg). This unique compound opens many new possibilities to new metallosilenes, disilabutadienes, sila–vinyl radicals, and other interesting reactive intermediates.

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