

Profile of Prof. Sason Shaik – recipient of the 2017 ICS Gold Medal

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Professor Sason Shaik

Professor Sason Shaik of the Hebrew University has been awarded the 2017 ICS Gold Medal together with Professor Yitzhak Apeloig of the Technion. Much has been written about Sason's achievements. In 2008, *The Journal of Physical Chemistry A* published a Festschrift in honor of his 60th birthday to which Sason contributed a fascinating autobiography based on a diary he had been keeping since 1979. In that year he returned to Israel after completing a PhD with Nicholas Epiotis of the University of Washington at Seattle and a postdoc with the Nobel prizewinner Roald

Hoffmann at Cornell University with whom he shares his love of art, poetry and chemistry. He also shares Hoffmann's originality and ability to see the same facts as others in a totally new light, and to go against the flow. In his autobiography, he describes himself as an "outsider" and as being "lucky" and "fortunate" in his scientific career.

Sason was born in Iraq in 1947 to a Jewish family. His father was a jeweler, as were many Iraqi Jews. His family left Iraq when he was a child due to the difficult security situation for Jews and immigrated to the newly established state of Israel. Life was hard in Israel for everyone but especially for new immigrants who were often sent to ramshackle transit camps. His family succeeded in moving out of the camp to Shkhu'nat Hatikva, a poor suburb in south Tel Aviv, and eventually to Ramat Gan where many Iraqis lived. Shortly afterwards, his father died and his mother raised him, together with his younger brother, single-handedly. Sason received a good education in the local school which encouraged and inspired gifted pupils. It was there that he developed his love of literature and writing. Later on, he added a love of chemistry and, in common with many budding chemists, performed risky experiments at home. The "magic of chemistry" had him in its grips. When he turned 15, he had to choose between humanities and literature and natural sciences. He chose science but one can see from his publications that his literary gifts have served him well.

After completing his army service in 1968, Sason began to study chemistry at Bar-Ilan University which was near his home. There, he first encountered "these creatures called orbitals" which led to a lifelong interest in theoretical chemistry. He describes the excitement of pushing arrows to determine a mechanism and learning how to decipher a spectrum. He was inspired by many of his teachers, especially Milon Sprecher, the founder of Bar-Ilan's chemistry department, whom he describes as a "rigorous teacher with a vast knowledge and a special gift for teaching." In 1972, after completing his BSc, he started an MSc in experimental tellurium chemistry with Michael Albeck. He found the experimental work hard and tedious but thoroughly enjoyed Milon Sprecher's course in molecular orbital (MO) theory which prompted him to start thinking about studying for his PhD in the USA. Towards

the end of his army service in the 1973 Yom Kippur war, while hiding from a missile attack in an Egyptian airfield, he suddenly understood the nature of the products that had so frustrated him in his experimental work and constructed an MO theory which led to his first publication.

His PhD studies with Epiotis and postdoc with Hoffman laid the foundations for his future scientific career and lifetime interest in valence-bond (VB) theory which at the time was thought to be inferior to molecular-orbital (MO) theory. Sason's first academic position was at Ben-Gurion University in Beer-Sheva where he rapidly established a fruitful collaboration with Addy Pross, a physical organic chemist. He flourished at Ben-Gurion and was eventually promoted to Full Professor. In 1991, he was invited to move to the Hebrew University of Jerusalem. His decision was aided by the outbreak of the Gulf War in 1991 which caused his Korean postdoc to flee the country. So despite many misgivings, he moved to Jerusalem in 1992 joining the institute of Chemistry as a Full Professor and also becoming a member of the Fritz-Haber Center for Molecular Dynamics which was established in 1981 with the help of the German Minerva Foundation. This gave him the idea of establishing a Center for Computational Quantum Chemistry funded by the Minerva Foundation. A proposal to set up the center was submitted by Sason and Yitzhak Apeloig of the Technion, the co-recipient of the 2017 ICS Gold Medal. In 1997, the center was inaugurated and called the Lise Meitner – Minerva Center for Computational Quantum Chemistry. Until its closure a year ago, its members derived from the Hebrew University, Technion, Tel-Aviv University, Weizmann Institute, Bar-Ilan University, and Ben-Gurion University, with Sason Shaik as director and Yitzhak Apeloig as co-director. Sason described his new life as director of the Center and mentor to a large research group as "I lost my freedom forever but, in retrospect, I gained a lot in return".

The scientific work of Sason Shaik has been wide-ranging, running the gamut from bonding in small molecules to the chemistry of metallo-enzymes. His work has renovated the map of chemical bonding, caused a paradigm shift in the understanding of aromaticity, and contributed new reactivity concepts, such as two-state and multi-state reactivities, which reoriented the fields of bioinorganic and metallo-enzymatic chemistry. Nevertheless, Sason considers the VB work to be his most important contribution. Sason is chiefly responsible for the renaissance of VB theory in modern times, and for its application to chemical bonding and chemical reactivity. The two "Shaik VB Diagrams" constitute a compact theory that applies all the way from the simplest reaction, $H\bullet + H_2$, to the complex hydrocarbon activation by P450 enzymes. The diagrams enable chemists to estimate activation barriers of elementary chemical steps "on the back of an envelope", to

predict changes in reaction mechanisms, to derive structural-selection rules for transition states, and to do this all across chemistry. On this choice, he likes to quote the following lines from Robert Frost's Poem, "The Road Not Taken":

"Somewhere ages and ages hence:
Two roads diverged in a wood, and I —
I took the one less traveled by,
And that has made all the difference."

In the mid-2000s, Sason developed ground rules for the usage of oriented external electric fields (OEEFs) as effectors of chemical change in nonpolar and non-redox reactions, and as a means of controlling reactivity and selectivity in reactions which involve the making and breaking of covalent bonds. His predictions were verified in an elegant set of experiments published in *Nature* in 2016. Quite a few groups of experimentalists have been inspired by the idea and have designed novel techniques to implement it. Shaik's seminal role in this surge of activity can be appreciated from the feature article written, on this emerging field, by the science journalist, J. Howgego in *Chemistry World* in January 2018. The area of OEEF control of nonpolar and nonredox chemical reactions has enormous fundamental value, limitless directions, and the potential to become a highly used smart technique. Sason's future plans are to focus on this area.

Sason is often asked by young scientists how to make their best choice in science. His short and simple answer is "Follow your hearts".

Arlene Wilson-Gordon was born in Glasgow, Scotland. She completed her BSc (Hons) at Glasgow University and her DPhil at Oxford University under the supervision of Peter Atkins. After a postdoc at the Hebrew University with Raphy Levine, she joined the faculty at the Department of Chemistry, Bar-Ilan University, where she rose to the rank of Professor and in 2015, Professor Emerita. Her research interests lie in the field of theoretical quantum and nonlinear optics. She is the editor of the *Israel Chemist and Engineer*, an online magazine for all who are interested in chemistry and chemical engineering.

