Professor Yaron’s research focuses on the theoretical description of the photophysics of conjugated polymers and other organic semiconductors. Describing the excited states of these systems poses an interesting and challenging problem in the electronic structure theory of large systems. Researchers in his group have also been developing new semi-empirical models by merging quantum chemical methods with machine learning. Current projects include: machine learning for chemistry, photophysics of disordered systems, and dyes for imaging biological systems.

Professor Yaron earned his doctorate at Harvard University, and was a post-doctoral fellow at the Massachusetts Institute of Technology. He joined the faculty at Carnegie Mellon University in 1992.

Neural nets are flexible tools that deep machine learning uses to recognize faces, win Go games, and drive cars. This talk will discuss two different applications of deep learning in chemistry. The first application uses a neural net to predict energy and other properties of molecules. The neural nets are first trained on a large set of data generated from accurate quantum chemical calculations. Once trained, the network can predict properties of new molecules in a fraction of the time required for the quantum chemical calculation. I will discuss the first deep learning method in which the neural net not only learns from the results of quantum chemistry, but does quantum chemistry as part of its prediction process. In the second application, we use neural nets to drive a reaction to a desired outcome. The neural net carries out thousands of experiments on a simulation of a polymerization reaction. Through trial and error, it learns to add catalysts and other reagents in a manner that leads to the desired distribution of polymer chain lengths.