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An activity portrait:

General:

I completed my Ph.D. in chemistry at Bar-Ilan University and received my Ph.D. in 1985. After receiving my doctorate, I continued to work at Bar-Ilan University in research with Prof. Avigdor Persky, my doctoral advisor, and at the same time in research with Prof. Rafi Levin from the Hebrew University as part of my postdoctoral fellowship.

Since 1992 I have been working at Ariel University (then called the Academic College of Judea and Samaria) as a visiting lecturer, and since 2002 as a faculty member in the Department of Chemical Sciences with the rank of senior lecturer. In 2016, I was promoted to associate professor.

My research focuses on exploring the mechanism of various processes. In the past, my research area was molecular dynamics. The research method was QCT – Quasi-Classical-trajectories – calculation of quasi-classical pathways. My research today deals with the computational chemistry of reactions using DFT (Density Functional Theory) using Gaussian software (g16) and VASP software.

I collaborate with researchers who do experimental work, Prof. Dan Meyerstein, Prof. Alex Shechter, Prof. Flavio Grynszpan**,** Dr. Tomer Zidki, Dr. Yael Albo, Prof. Mindy Levin, from the university and Prof. Ariella Borg and others from outside.

My teaching focuses mainly on theoretical courses: quantum chemistry, molecular spectroscopy, and mathematical modeling in chemistry. In this context, I wrote an online textbook on quantum chemistry based on my lectures.

In addition to my teaching and research activities, I served as Head of the Department of Chemical Sciences from 2015 to 2021. Starting in 2022, I serve again as chair of the department's teaching committee. Since 2022 till now, I have been also a member of the regulation committee of Ariel University. In the past, I was a member of other committees: the student disciplinary committee and the library committee.

Research activity

My study is focused on homogeneous catalysis and heterogeneous catalysis. The results of my research have been published in about 60 publications in leading journals. and at several conferences.

Main research topics:

a. Homogeneous catalysis:
   - The Fenton reaction, in which hydrogen peroxide oxidizes tartaric acid in an aqueous solution with Fe(II) ions as a catalyst was published in 1894. This reaction participates in "oxidative stress" processes in the body, and it contributes to aging processes and various diseases. Although this reaction has been extensively studied, there is no agreed mechanism for it. Thorough DFT research was done to understand which factors affect

this process. The role of carbonate ions as a cocatalyst while a transition metal is used as a catalyst was revealed.

- Although metallic nanoparticles have important roles in chemistry and engineering, and it is very easy to produce them in the lab, the mechanism of their production is unclear. According to thermodynamics, it seems as if their production in a bottom-up mechanism is forbidden. A detailed computational study revealed the mechanism of the production of silver and gold nanoparticles from the cations.
- Key Intermediates, Omitted Mechanisms, and Unsymmetrical Bimane Products were explored in a solution of CH_2Cl_2.

b. Heterogeneous catalysis

- Nanoparticles act as catalysts for various reactions; we focused on BH4-hydrolysis reaction and hydrogen release on silver and gold nanoparticles. In this study, it was necessary to calculate the energy of an adsorbed ion on a metallic surface – a charged system. Such a calculation is, in principle, impossible in VASP. We developed and published the counter-ion method that enables such calculations.
- Hydrogen evolution is explored on other transition state metals.
- Due to the global energy crisis and environmental demands, fuel cells attract a lot of attention. To enable the usage of fuel cells, inexpensive catalysts with a reduced amount of Pt and new-generation fuels are required. Using DFT calculations, we investigate the oxidation of several fuels: methanol, dimethyl ether, formic acid, and methyl format using Pt alloys (bimetallic and ternary) as catalysts. The role of each metal in the alloy was explored. this information is supposed to enable the design of an ideal alloy for oxidizing a given fuel.

Future plans:

In the coming years, I intend to continue my research and teaching work in the Department of Chemical Sciences. The topics I plan to explore are:

a. Study of reactions on nanoparticles - The reactions that will be investigated are of great environmental importance. De-halogization of haloalkanes, which are dangerous toxins, pollute water sources and seas and damage the ozone layer. Such processes should be investigated computationally to avoid the usage of hazardous materials.
b. Reaction of radicals on the surfaces, e.g. methyl radical will be explored.
c. Fuel cell- research will continue and be extended to ORR (oxygen reduction reaction) and carbon-free fuels.
d. single atom catalyst - The reduction of carbon dioxide will be explored on a graphite surface with a single copper atom bound to it.