

# Princeton University

Honors Faculty Members  
Receiving Emeritus Status



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The biographical sketches were written by colleagues in the departments of those honored, except where noted.

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# Zoltán G. Soos



Zoltán Soos arrived in Princeton as an assistant professor of chemistry in 1966, having completed both his graduate studies and a postdoctoral year with Harden McConnell over two years at the California Institute of Technology and two at Stanford University. McConnell was interested in triplet spin excitons in salts of “TCNQ,” which were new materials that were based on stacks of planar anions, each with a single unpaired electron. At a time when the electronic structure of organic solids was largely unexplored, Zoltán’s projects were to devise solid-state theoretical, as opposed to computational, models for TCNQ salts and their spin resonance spectra. Later, his studies came to include conducting organic materials such as “TTF-TCNQ” and organic superconductors.

Zoltán’s research at Princeton continued at that frontier between chemistry and physics that he helped pioneer, focusing on organic solids, donor and acceptor species, conjugated polymers, and linear spin systems. With his first graduate student, Paul Strebel, and his first postdoctoral associate, Doug Klein, Zoltán modeled both optical and magnetic excitations for salts of the acceptor species TCNQ. Indeed, these original studies of his gave rise to a simple, elegant classification of TCNQ, TTF, and related salts in terms of stoichiometry, type of stacking, and repeat unit along the stack. He proposed that high conductivity in organic solids was decisively related to less than or more than half-filled bands, as had been previously proposed for a hypothetical chain of H atoms.

Together with his students Sumit Mazumdar and Steve Bondeson, Zoltán developed a diagrammatic valence bond (VB) theory that facilitated an exact solution of finite correlated models for neutral-ionic transitions or for spin chains with random weak links. This approach to VB theory became enormously powerful when his colleague S. Ramasesha showed that the linear combination of Slater determinants in each

diagram could be uniquely encoded as an integer; large configuration-interaction problems could then be done on workstations.

Conjugated organic polymers rose to prominence in the 1980s with reports on polyacetylene as a conductor; other conjugated polymers are insulators with large nonlinear optical (NLO) responses. Zoltán furthered research in this field with collaborators including Ramasesha, Peter McWilliams and Geoff Hayden, and Shahab Etemad at Bellcore. Zoltán also had a longstanding collaboration with Anna Painelli and Alberto Girlando at the University of Parma. With Sharon Bewick, Zoltán worked out the differences between thermally induced and quantum transitions in the electronic ground state, and together quantitatively modeled the spin-Peierls transition of a TTF<sup>+</sup> salt.

Research in closed-shell organic solids has burgeoned in recent years, thanks to academic and commercial interest in organic electronic devices based on thin films that mitigate low conductivity based on a hopping mechanism for transport of charges that are localized on molecules. Zoltán and Eugene Tsiper formulated a practical self-consistent treatment of electronic polarization based on the idea that electrostatic potentials at atoms are easily incorporated in semi-empirical theory. This method could be adapted to thin films where it accounted well for photoelectron and inverse photoelectron spectra, as measured by Antoine Kahn's group in electrical engineering. Zoltán determined that electronic polarization could be combined with molecular potentials to model the ionization potential of films in which the individual molecules were either "lying down" or "standing up" with regard to a substrate, or to model scanning tunneling microscopy spectra of pentacene films containing surface and subsurface dopants.

Spin chains of transition metal ions are another area of recent interest to which Zoltán has made fundamental theoretical contributions in collaboration with his chemistry department colleagues Pascal and Bob Cava, Manoranjan Kumar, and Sian Dutton.

In addition to his extensive collaborative network that is centered in Princeton, Zoltán spent six productive summers and a sabbatical leave (between 1967 and 1989) at the Sandia National Laboratories in Albuquerque, New Mexico. It is not entirely clear whether it was study-

ing electron spin resonance in CT salts, or the distinctive signature of spin dynamics of linear systems (with Bob Hughes), or  $\sigma$ -conjugated polysilanes (with Glen Kepler), or rather the beautiful scenery, excellent climate, and marvelous cuisine of Northern New Mexico that kept luring him back to Sandia.

Research on organic solids and spin chains has proven to be especially rewarding for Zoltán: organic electronics is now a large and thriving enterprise. Characteristically modest, he says he was fortunate to start when the field was young; practitioners in this area might counter that statement replying that it was the field that was fortunate to have had him, as one of its groundbreaking intellectual leaders, when it was in its infancy. It is not surprising, therefore, that a colleague remarks, “Zoltán’s work is distinguished by the physical insight into the electronic properties of organic solids and thin films that it provides. His formal, theoretical approach, based on simple, elegant models of very complex systems (in contrast to brute force computational approaches to these questions) has put the field of the electronic structure of organic solids on a firm fundamental foundation. This foundation has truly enabled the broad application of organic materials in modern electronic devices.”