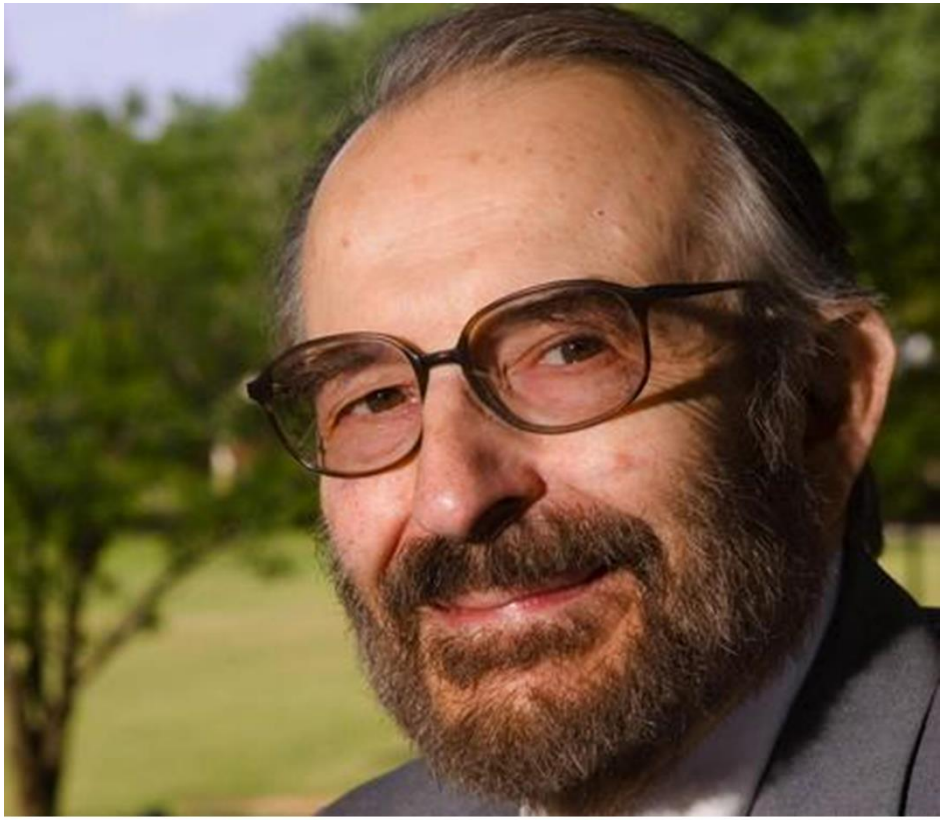

Theory and Experiment: A Meeting at the Interface

Erlangen, 30th March – 1st April 2016

molecular graphics modelling society

WILEY

GDCh Gesellschaft Deutscher Chemiker

FCI Fonds der Chemischen Industrie

Program

(all lectures will be in the Großer Hörsaal, Organic Chemistry, Henkestraße 42)

11:00 onwards	**Registration, Foyer, Organic Institute, Henkestrasse 42**		
Wed., March 30th		**Opening**	**Tim Clark**
13^{00}	Tim Clark	*Welcome and Introduction*	
13^{10}	Helmut Schwarz	*Thermal Hydrogen-Atom Transfer from Methane: A Mechanistic Exercise*	
		Princeton and the early days	**Peter Stang**
14^{00}	Robert Glaser	*A Perfect Pair: Cucurbit[7]uril/Diamantane Guest with an Attomolar Dissociation Constant*	
14^{25}	Jörg Daub	*From degenerate Carbocations to light-stimulated Processes*	
14^{50}	Pierre Laszlo	*Paul and Princeton, My Recollections*	
15^{15}	Volker Buss	*In Search of Lost Time - 3 Years as Graduate Student in Princeton*	
		Coffee	
16^{30}	Yitzhak Apeloig	*From the Norbornyl Cation to Planar Carbon and to Silicon Chemistry*	
16^{55}	Leo Radom	*My Interactions with Paul Schleyer: Early Days in the Transformation to Computational Chemistry, and Beyond*	
17^{20}	Eluvathingal Jemmis	*Transitions: Princeton, Munich and Erlangen*	
17^{45}	Peter Stang	*A biological Self-Assembly: Predesigned Metallacycles and Metallacages via Coordination*	
18:10	**Mixer and Get-Together, Foyer, Organic Institute, Henkestrasse 42**		

Thur., March 31st	Erlangen (1)	Herbert Mayr
9[00]	Rolf Saalfrank	*Progress is linked to the past - Calculated or made: what´s the difference?*
9[20]	Rainer Herges	*Photoswitchable Molecular Magnets and Their Application in Medical Imaging*
9[45]	Ernst-Ulrich Würthwein	*Where is the nodal plane? The search for highly reactive nitrogen intermediates*
10[10]	Matthias Bickelhaupt	*Aromaticity and Antiaromaticity: MO Picture of Intuitive Concepts*
		Coffee
11[15]	Holger Bettinger	*Polycyclic aromatics*
11[40]	Hans-Ullrich Siehl	*From superacid chemistry to ´in silico´ chemistry*
12[05]	Matthias Bremer	*Liquid-crystal research in Merck*
12[30]	Alexander Kos	*iScienceSearch - the "Google" for Chemists*
		Lunch

	Erlangen (2)	Ernst-Ulrich Würthwein
14[15]	Pavel Hobza	*The recent view on non-covalent interactions*
14[40]	Yun-Dong Wu	*Theoretical Studies of catalytic C-H bond activation reactions*
15[05]	Martin Kaupp	*Quantum-chemical insights on mixed-valence systems*
15[30]	Andy Streitwieser	*Organolithium Chemistry*
		Coffee
16[30]	Michael Bühl	*NMR chemical shift calculations*
16[55]	Ulrike Salzner	*Predicting Absorption Spectra of Large Conjugated π-Systems*
17[20]	Koop Lammertsma	*Physical Organic Chemistry – the P-C connection*
17[45]	Herbert Mayr	*A quantitative approach to polar organic reactivity*

Fri., April 1st	Current Erlangen colleagues	Tim Clark
9[00]	Ralph Puchta	*Computational Coordination Chemistry*
9[20]	Johann Gasteiger	*Chemoinformatics - Learning from Chemical Data*
9[45]	Sjoerd Harder	*The Development of Organocalcium chemistry - From Metallocenes to Applications*
10[10]	Karsten Meyer	*Crystal Structure Determination of the Nonclassical 2-Norbornyl Cation*
		Coffee
11[15]	Andreas Hirsch	*Spherical Aromaticity*
11[40]	Rik Tykwinski	*Can synthesis challenge theory?*
12[05]	Tim Clark	*Can theory challenge synthesis?*
12[30]	Walter Bauer	*Classical NMR and classical music: missing link and missing Paul*
		Lunch

Fri., April 1st	University of Georgia	Fritz Schaefer
14[15]	Gernot Frenking	*Molecules With and Without Unusual Bonds: Research in the Spirit of Paul Schleyer*
14[40]	Judy Wu	*Aromaticity-Modulated Hydrogen Bonding: Making Weak Acids Strong Proton Donors*
15[05]	Wesley Allen	*Troublemaking with Paul Schleyer: Iconoclastic research on vibrational spectra and SN2 reactions*
		Coffee
16[15]	Jürgen Gauss	*New Molecules via the Interplay of Theory and Experiment*
16[40]	Clemence Corminboeuf	*Putting Forward Replica Exchange Molecular Dynamics and Other Tools for Computational Organic Chemistry*
17[05]	Peter Schreiner	*London Dispersion in Molecular Chemistry—Reconsidering Steric Effects*
17[30]	Fritz Schaefer	*Density Cumulant Functional Theory*
17[55]	Fritz Schaefer	*Closing Remarks*