In 1963, before become „transistorized”, Dr Csizmadia used a vacum-tube computer at M.I.T., an IBM 709, to perform the very first Gaussian Quantum Molecular Computation on an organic molecule (HCOF). With this trailblazing accomplisment, the field of organic chemistry become computational. This achievement resulted in the science of chemistry changing from an „empirical” to an „exact” science. Since that time, he has published more than 500 research papers and 13 scientific books.

SZEGEDI TUDOMÁNYEGYETEM
JUHÁSZ GYULA PEDAGÓGUSKÉPZŐ KAR

50th anniversary of the first ab initio calculations on organic molecules

1963-2013

Meghívó

Programme
10/28/2013

		Minnutes
11:00-11:10	*Gábor Szabó: Opening remarks of the Rector*	10
11:10-11:20	*Béla Viskolcz: 50 years of ab initio calculations*	10
11:20-11:30	*Introduction*	10
11:30-12:00	*Imre G. Csizmadia: Past and future of mathematical models*	30
12:00-12:30	***Coffee break***	30
12:30-13:00	*Lévai Péter: Challange of "Big Data"*	30
13:00-13:30	*András Perczel: Protein folding*	30
13:30-14:00	*Birgit Strodel: Simulation of protein aggregation: The molecular basis for Alzheimer's disease*	30
14:00-14:30	*Sarah Harris: Architecture of bio structure*	30
14:30-14:45	***Coffee break***	15
14:45-15:15	*Svend K. Jensen: Chemistry as a computable exact science*	30
15:15-15:45	*Martinek Tamás: Future of drug discovery process*	30
15:45-16:15	*Attila Császár: 4th age of quantum chemistry*	30
16:15-:16:45	***Coffee break***	15
16:45-17:00	*Imre Jákli: Torus representations of Ramachandran surfaces*	30
17:00-17:30	*Zoltán Mucsi: Systems chemistry*	30
17:30-18:00	*Béla Viskolcz: Challanges of Education*	30
18:00~	*Imre G. Csizmadia: Supper & Round Table Discussion: New way of teaching: CREATIVITY*	30 ~
Posters:	*Anita Rágyanszki*	
	Attila Surányi	
	Balázs Roósz	
	János Szórád	
	Selma Yarligan Uysal	

Programme
10/29/2013

		Minnutes
9:00-9:30	*Botond Penke: Misfolded proteins in Alzheimer*	30
9:30-10:00	*Zoltán Kónya: Challange of discovery of new materials*	30
10:00-10:30	*Norbert Búzás: Future of innovation*	30
10:30-10:45	***Coffee break***	15
10:45-11:00	*Szilárd Fejér: Coarse-grained modelling of amyloid*	15
11:00-11:15	*Balázs Jójárt, Béla Fiser: Glutathione - radical recognition process*	15
11:15-11:30	*Babak Minofar: Biomolecular simulations in non-aqueous media*	15
11:30-11:45	*David Řeha: Application of QM/MM calculations in biological systems*	15
11:45-12:00	*Milán Szőri: Evolution at molecular level*	15
12:00-12:15	*Cimino Franco Prado Andreas: Relative stability of selected biobricks*	15
12:15-12:30	***Coffee break***	15
12:30-12:45	*Michael Owen: The effects of hydrogen abstraction on peptide structures*	15
12:45-13:00	*Klára Gerlei: Atropisomerism of Asn a radicals*	15
13:00:13:15	*Natalie Galant: Theoretical study of disulfid bridges*	15
13:15-13:30	*István Mándity: High performance organocatalytic transformations in continuous flow*	15
13:30~	*Imre G. Csizmadia: Closing remarks*	~

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„Tudástár" lecture room