# Curriculum Vitae of SANDOR KRISTYAN



Budapest (Hungary), 1955, married, 2 children Born Office address Hungarian Academy of

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## **EDUCATION AND EMPLOYMENT HISTORY**

Education	1975 – 1980	B.S.(1978), M.S.(1980) in Chemical Engineering, Faculty of medicine, Budapest University of Technology, Budapest, Hungary
	1979-1988	M.S.(1988) in Mathematics, Eotvos Lorand University TTK, (evening class), Budapest, Hungary
	1980-1982	D.Sc.(1986) in Physical Chemistry, Hung.Acad.Sci. Institute of Isotopes, Budapest University of Technology, Budapest, Hungary
	1983-1985	Ph.D.(1985 ) in Mathematical Sciences in Chemistry, University of Texas at Arlington, Department of Chemistry, Arlington, Texas, USA
Employment	1986-1989	Budapest University of Technology, Institute of Physics, Budapest, Hungary, Department of Atomic Physics, Surface Sciences Laboratory, Department engineer and research associate
	1989-1990	Baylor University, Department of Chemistry, Waco, Texas, USA, Postdoctoral fellow
	1990-1992	California Institute of Technology, Division of Chemistry and Chemical Engineering, Pasadena, CA, USA, Postdoctoral fellow, Advisor: Prof. Aron Kuppermann
	1992-1993	Illinois Institute of Technology, Chemical Engineering Department, Chicago, Illinois, USA, Senior Research Associate
	1993-1995	University of Arkansas, Department of Chemistry and Biochemistry, Fayetteville, Arkansas, USA, Research Instructor, Advisor: Prof. Peter Pulay
	1995-1997	Emory University, Department of Chemistry, Atlanta, GA, USA, Senior Postdoctoral Research Associate
	1998 summer	Budapest University of Technology, Department of Inorganic Chemistry, Budapest, Hungary, Domus Hungarica Visiting Professor
	1998-1999	Emory University, Department of Radiation Oncology, Division of Cancer Biology, Atlanta, GA, USA, Research Associate
	1999 summer	Budapest University of Technology, Department of Inorganic Chemistry, Budapest, Hungary, Domus Hungarica Visiting Professor
	1999-2000	George Washington University, Department of Chemistry, Washington, DC, USA, Lecturer in Physical Chemistry
	2001-present	senior research fellow, Institute of Materials and Environmental Chemistry,

Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary

#### **FIELDS OF INTEREST**

Present: computation chemistry (ab initio, density functional theory),

molecular mechanics, molecular dynamics, molecular modelling,

modelling lipid bi-layers, surfaces properties and diffusion, potential energy surfaces,

synthetic organic chemistry and medicine,

numerical methods in chemistry

Former: heterogeneous catalysis (hydrogenolysis and poisoning of ethane on Ni and Pd),

transport processes (segregation and diffusion to the metal surfaces from the bulk),

metal surfaces,

collision between atoms and surfaces

General training in: Physical chemistry,

theoretical/quantum chemistry,

biophysics, physics,

thermodynamics, statistical mechanics,

reaction kinetics and dynamics,

mathematics

Extensive experience in computer programming:

Software: Spartan 2006 and higher,

Gaussian 98/DFT and higher,

Schrodinger/Maestro,

Cerius2, Gromacs,

Systems: LINUX (UNIX),

FORTRAN,

PC (Windows, Office, Origin, etc.), Macintosh,

www

#### **GRANTS, FELLOWSHIPS**

1998 & 1999 Budapest University of Technology, Department of Inorganic Chemistry, Budapest,

summer Hungary, Domus Hungarica Visiting Professor

2007-2009 Hungarian Research Grant OTKA-2007, 2 years, K-68293

### MEMBERSHIPS, PROFESSIONAL SERVICES

1983 – 1985 Member of the American Chemical Society

**TEACHING EXPERIENCE** 

1986-1989 Budapest University of Technology, Institute of Physics, Budapest, Hungary,

University Physics teaching

1999-2000 George Washington University, Department of Chemistry, Washington, DC, USA

Lecturer in Physical Chemistry

**LANGUAGE** 

Hungarian (native language), English (write, speak, lecture)