## **Stavros C. Farantos**

Professor of Theoretical Chemistry and Affiliated Research Scientist in IESL-FORTH

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## **Education & Work experience**



Born	: June 3rd, 1951, Piraeus.
October 1969 - June 1973	: First degree in Chemistry,
	Department of Chemistry, University of Athens.
October 1973 - February 1976	: Military service.
April 1976 - September 1978	: Ph. D. degree in Theoretical Chemistry,
1 1	University of Sussex (Title :
	Potential Energy Surfaces and Molecular
	Dynamics of Chlorine - Oxygen system
	Supervisor: Professor John N. Murrell (FRS).
October 1978 - October 1981	Research Fellow, School of
	Molecular Sciences, University of Sussex.
November 1981-September 19	84 : Research Scientist, Theoretical and
1	Physical Chemistry Institute, National
	Hellenic Research Foundation.
October 1984 - July 1989	:Assistant Professor in Chemistry,
5	University of Crete, and Research
	Scientist in the IESL, Foundation for
	Research and Technology-Hellas.
July 1987 - September 1987	: Visiting Researcher, Department of
2	Chemistry, University of Bielefeld, Germany.
July 1989 - June 1990	: Visiting Professor, Departments of
5	Chemistry and Physics, University of
	Southern California, California, USA.
August 1989 - March 1994	: Associate Professor in Chemistry,
2	University of Crete, and Research
	Scientist in IESL, Foundation for
	Research and Technology-Hellas.
April 1994 - Present	: Professor in Chemistry,
Ĩ	University of Crete, and Research
	Scientist in IESL, Foundation for
	Research and Technology-Hellas.

## **Research interests**

- [1] Spectroscopy, dynamics and thermodynamics of atomic and molecular clusters.
- [2] Theoretical vibrational spectroscopy of small polyatomic molecules with atmospheric interest.
- [3] Elementary chemical reactions isomerization, dissociation in small polyatomic molecules.

Applications of nonlinear mechanics.

- [4] Energy localization and redistribution in biological molecules.
- [5] Development of methods and computer codes for novel high performance, high throughput computational schemes - Grid & Cloud computing - for classical and quantum dynamics.

## **Representative publications**

[1] Vangelis Daskalakis, Stavros C. Farantos, and Constantinos Varotsis. Assigning vibrational spectra of ferryl-oxo intermediates of Cytochrome c Oxidase by periodic orbits and Molecular Dynamics.

J. Am. Chem. Soc., 130(37):12385 12393, 2008.

[2] Stavros C. Farantos, Reinhard Schinke, Hua Guo, and Marc Joyeux. Energy Localization in Molecules, Bifurcation Phenomena, and their Spectroscopic Signatures: The Global View.

Chemical Reviews, 109(9), 4248-4271, 2009.

[3] Jaime Suarez, Stavros C. Farantos, Stamatis Stamatiadis, and Lucas Lathouwers. A method for solving the molecular Schroedinger Equation in Cartesian coordinates via angular momentum projection operators.

Comp. Phys. Comm., 180:2025-2033, 2009.

[4] Massimiliano Porrini, Vangelis Daskalakis, S. C. Farantos, and Constantinos Varotsis.
Heme Cavity Dynamics of Photodissociated CO from ba3-Cytochrome c Oxidase: the Role of Ring-D Propionate.
J. Phys. Chem. B, 112, 12120, 2000.

J. Phys. Chem. B, 113, 12129, 2009.

[5] R. Schinke, J. Suarez, and S. C. Farantos.Photodissociation of N2O: Frustrated NN bond breaking causes difuse vibrational structures.J. Chem. Phys. (Communication), 133, 091103, 2010.