NANOSCIENCE AND NANOTECHNOLOGY PROGRAM

Patrizia Calaminici, Ph.D.

Research:

Applications and developments within the framework of density functional theory and we are currently focusing on the following research topics:

- Temperature dependent properties of finite systems (Polarizabily, Heat Capacity)
- Ab-initio Born-Oppenheimer molecular dynamic (BOMD) simulations
- Metals and transition metal clusters
- Endohedral and large fullerenes
- Biological systems

Dr. P. Calaminici is professor of the Department Chemistry. She received a bachelor degree in Physics (Theoretical Physics) and a Ph.D. degree in Chemistry (Inorganic Chemistry) from the University of Calabria (UNICAL), Italy. During her Ph.D. studies Dr. Calaminici spent 18 months (Jul. 1993-Dec.1994) as research assistant at the University of Montréal in the research group of Dr. D.R. Salahub. She returned to Italy, completed her Ph.D. thesis and defended it in 1996 at the University La Sapienza, in Rome, Italy. She moved than for a post-doctoral position to the University of Hannover, Germany, from 1997 to Sep. 1999. Since Sep. 1999 she is full professor at the Chemistry Department of Cinvestav, working in theoretical chemistry. Dr. Calaminici has received different grants to develop her research. She has supervised different Ph.D., Master and undergraduate students as well as she has received several post-doctoral fellows have been associated to her research group. Dr. Calaminici is author of about 90 peer reviewed articles and of more than 10 book chapters. These works together have received more than 2000 citations. She is co-author of the deMon2k code which is currently used by about five hundred research groups all around the world. The research group of Dr. Calaminici has established active collaboration with several research groups from abroad and within Mexico.

Selected Honours and Awards

- Level III in the SNI.

Research Project for Nanoscience and Nanotechnology:

Development and applications within density functional theory in order to determine different properties such as ground state structures, transition state structures, frequencies, energy properties, optical and magnetic properties of complex systems relevant in the field of nanoscience and nanotechnology like transition metal systems, endohedral fullerenes and biological systems. The classes of systems to be investigated are selected on depending of the interest of the Ph.D. candidates and on the basis of their background. These studies will be performed with density functional theory. The proposed Ph.D. project aims to bridge theoretical results with experimental data in order to elucidate the molecular structure of the studied complex systems, to determine their relevant energy properties (binding energy, ionization potential, electron affinity etc.), to evaluate properties such as electric properties (dipole moments, polarizabilities, hyperpolarizabilities, etc.) or magnetic properties (magnetic moments, chemical shift, etc.) and to understand the elementary steps in chemical reactions of which the considered complex systems classes are involved.