Nonlinear Double Day 2005 Continuation Nonlinear excitations: theory and experiments Organized by **GFNL**, the **Group of Nonlinear Physics** of the University of Sevilla (http://www.grupo.us.es/gfnl) With the collaboration of the Department of Applied Physics I Friday, April 1, 2005. 11.30

Molecular Modelling of Nucleic Acids:

How Quantum Chemistry Might Help?

Speaker: Eugen Starikov

Seminar of the **Department of Applied Physics I at ETSI Informática** (L3). Avda Reina Mercedes s/n, 41012-Sevilla, Spain

Abstract:

The following aspects of theoretical chemical physics of nucleic acids will be discussed:

- 1. Frontier orbitals in DNA
- 2. Nature of electronic excited states in DNA
- 3. Nature of disorder in DNA
- 4. Electron-phonon coupling in DNA
- 5. Electron correlations in DNA
- 6. DNA doping

The talk will try to clarify the role of quantum-chemical investigations in tackling the above 6 topics.

Dr. **Starikov**, from Ukraine, currently at the Institut for Theoretic Solid State Physics, University of Karlsruhe, Germany, has been working in the above and related topics with leading scientists as Wolfram Saenger, Hans Lehrach, Director of the German branch of the Human Genome Project, Max F. Perutz, Nobel Prize Laureate, and his colleague Alan Windle.

Organizer: Juan FR Archilla