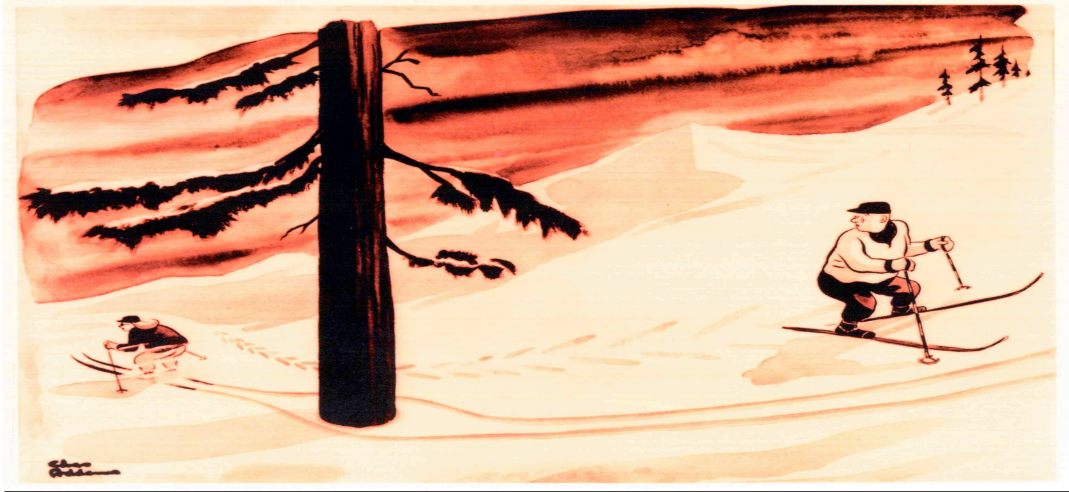


QUANTUM SEMINARS

Physics Dept. Theory Section,
University of Trieste



Fabio Pichierri

Professor of Chemistry, School of Engineering, Tohoku University

All-Atom quantum mechanical studies of proteins

May 15th , 16:30 PM, Seminar Room 204, ICTP building.

In this talk I will present the results of all-atom quantum mechanical calculations of proteins. These calculations, in spite of being approximate, shed light on the electronic structure of proteins, particularly on the distribution of the electronic charge throughout the whole molecule. Further, the electric dipole moment of the protein represents an important property which can be correlated to biological processes as different as molecular recognition and signal transduction