

The Theoretical and Computational Chemistry Group (TCCC) contribution to FuturICT

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- ▶ Theoretical vibrational spectroscopy of small polyatomic molecules with atmospheric interest.
- ▶ Elementary chemical reactions - isomerization, dissociation - in small polyatomic molecules. Applications of nonlinear mechanics.
- ▶ Energy localization and redistribution in biological molecules.
- ▶ Development of methods and computer codes for novel high performance computational schemes - Grid computing - for classical and quantum dynamics.

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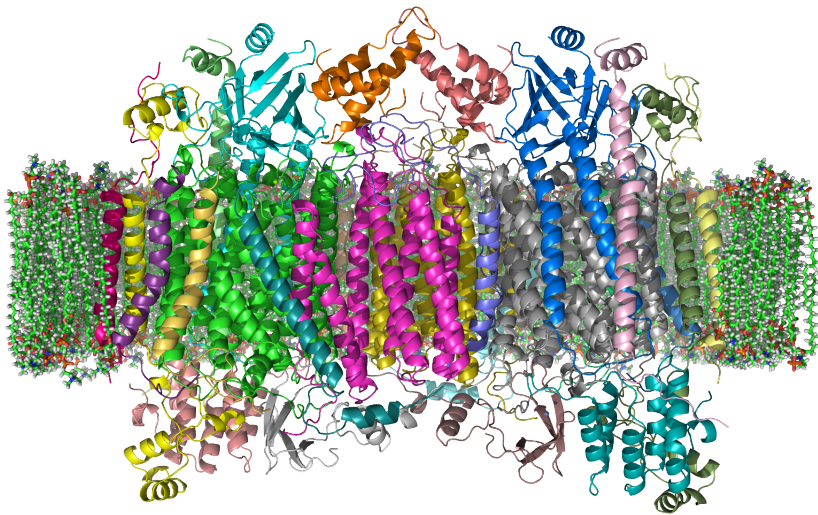
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Chemical Complex Systems



GRID COMPUTATIONAL CHEMISTRY COMMUNITY (GC3) FOR STUDYING COMPLEXITY IN GLOBAL ENVIRONMENTAL PROBLEMS AND EDUCATION

A sketch proposal for FuturICT

The aim of the proposal is to design, implement and exploit cooperative/competitive ICT instruments as working tools for developing a seminal Virtual Research Community (VRC) operating on Complex Systems of the Planetary Nervous System, focus area of FuturICT, to successfully tackle some grand challenges in the application areas of technology, environment and education.

Some possible projects

- ▶ DESIGN AND IMPLEMENTATION OF USER FRIENDLY TOOLS FOR MOLECULAR SCIENCE VIRTUAL COMMUNITIES
- ▶ DEVELOP A GRID EMPOWERED MOLECULAR SIMULATOR
- ▶ ENHANCE TECHNOLOGY TRANSFER: CLEAN COMBUSTION MODELING
- ▶ BUILD MANAGEMENT TOOLS FOR GOVERNING COMPLEX SYSTEMS PROVIDING SERVICES OF HIGH SOCIAL IMPACT: CHEMISTRY BASED STORAGE OF RENEWABLE ENERGIES
- ▶ DISTRIBUTED MANAGEMENT OF MOLECULAR SCIENCE VIRTUAL CAMPUS AND LEARNING OBJECTS

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Organizers and Potential Collaborators

- ▶ **Stavros Farantos (*)**, IESL/FORTH and University of Crete, Greece,
- ▶ **Antonio Lagana (*)**, University of Perugia, Italy,
- ▶ **Oswaldo Gervasi**, Dept. Math & Comp Science, University of Perugia, Italy
- ▶ **Sergio Maffioletti**, Grid Computing Competence Center - University of Zurich, CH
- ▶ **Domenico Laforenza**, IIT, Pisa, Italy
- ▶ **Frederique Battin-Leclerc**, Université de Nancy, France
- ▶ **Ernesto Garcia**, University of the Basque Country, Spain
- ▶ **Francesco Esposito**, PLC Systems SpA, Napoli, Italy
- ▶ **(*) Organizers**