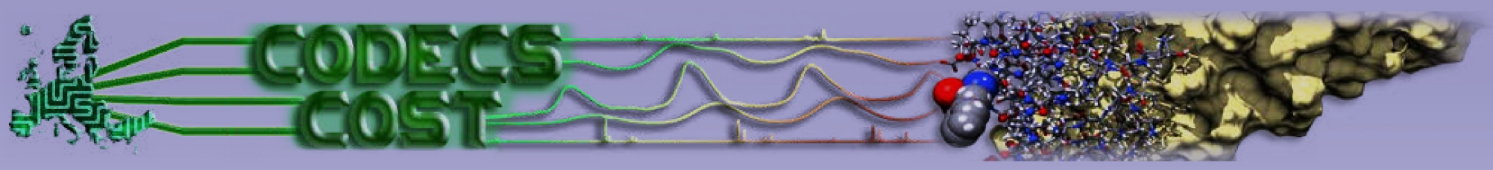
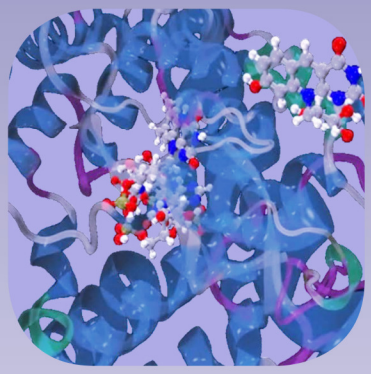
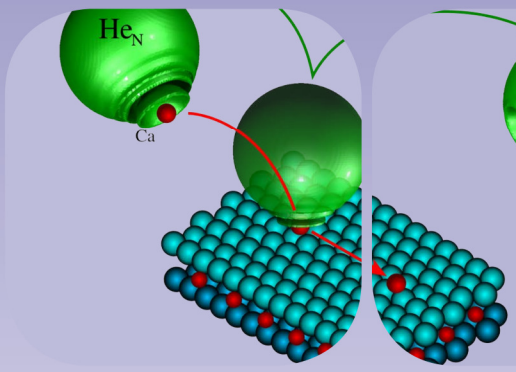
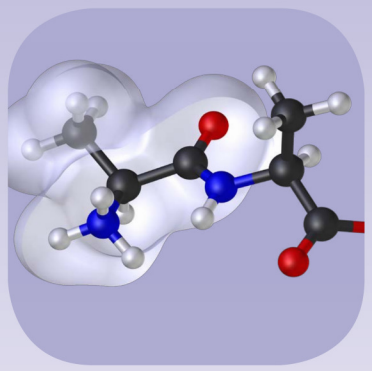




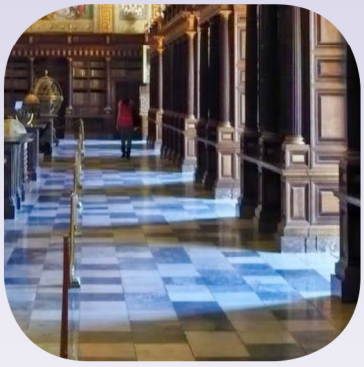


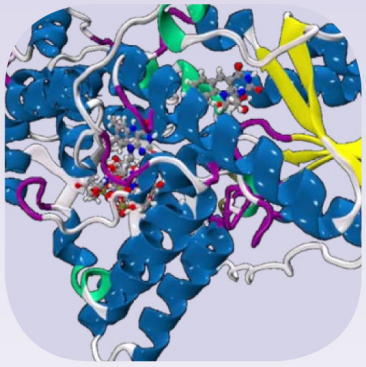
APRIL 18-22
2013

CODECS 2013
WORKSHOP



San Lorenzo
de El Escorial
Madrid
(SPAIN)





CONVERGENT DISTRIBUTED ENVIRONMENT FOR COMPUTATIONAL SPECTROSCOPY

TOPICS

- Spectroscopy and charge-transfer processes at molecule-surface interfaces with density functional theory and beyond
- Theoretical descriptions of complex solvent environments with macroscopic (continuum) and microscopic approaches: Spectroscopy and Soft-landing
- Mixed QM/MM and large-scale quantum simulations of biological and photobiological mechanisms
- Highly accurate spectroscopy and control of molecular systems including wide-amplitude (highly anharmonic) nuclear motions, van der Waals interactions and EM fields
- Partitioning, embedding and multi-scale simulations of complex systems and spectroscopic implications
- Highly accurate spectroscopic descriptions bridging the gap between small molecules/complexes and molecular systems of biological relevance/bulk materials
- Challenging design of novel materials and molecular complexes from ab-initio simulations for optical and spectroscopic applications
- Theoretical modeling of electro-magnetic spectroscopic properties

ORGANIZING COMMITTEE
MARÍA PILAR DE LARA-CASTELLS | Instituto de Física Fundamental, IFF-CSIC, Madrid (SPAIN) - CHAIR
JOSÉ CAMPOS MARTÍNEZ | Instituto de Física Fundamental, IFF.CSIC, Madrid (SPAIN)
MAR REGUERO DE LA POZA | Universidad Rovira i Virgili, Tarragona (SPAIN)
MALGORZATA BICZYSKO | Scuola Normale Superiore, Pisa (ITALY)

SCUOLA NORMALE SUPERIORE

cost
EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

GOBIERNO DE ESPAÑA · MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

UNIVERSITAT ROVIRA I VIRGILI

Elaborazione a cura del Servizio Comunicazione e Relazioni Esterne | SNS

http://fama.iff.csic.es/con/COST2013/codecs2013.htm
Email: iff_codecs2013@iff.csic.es