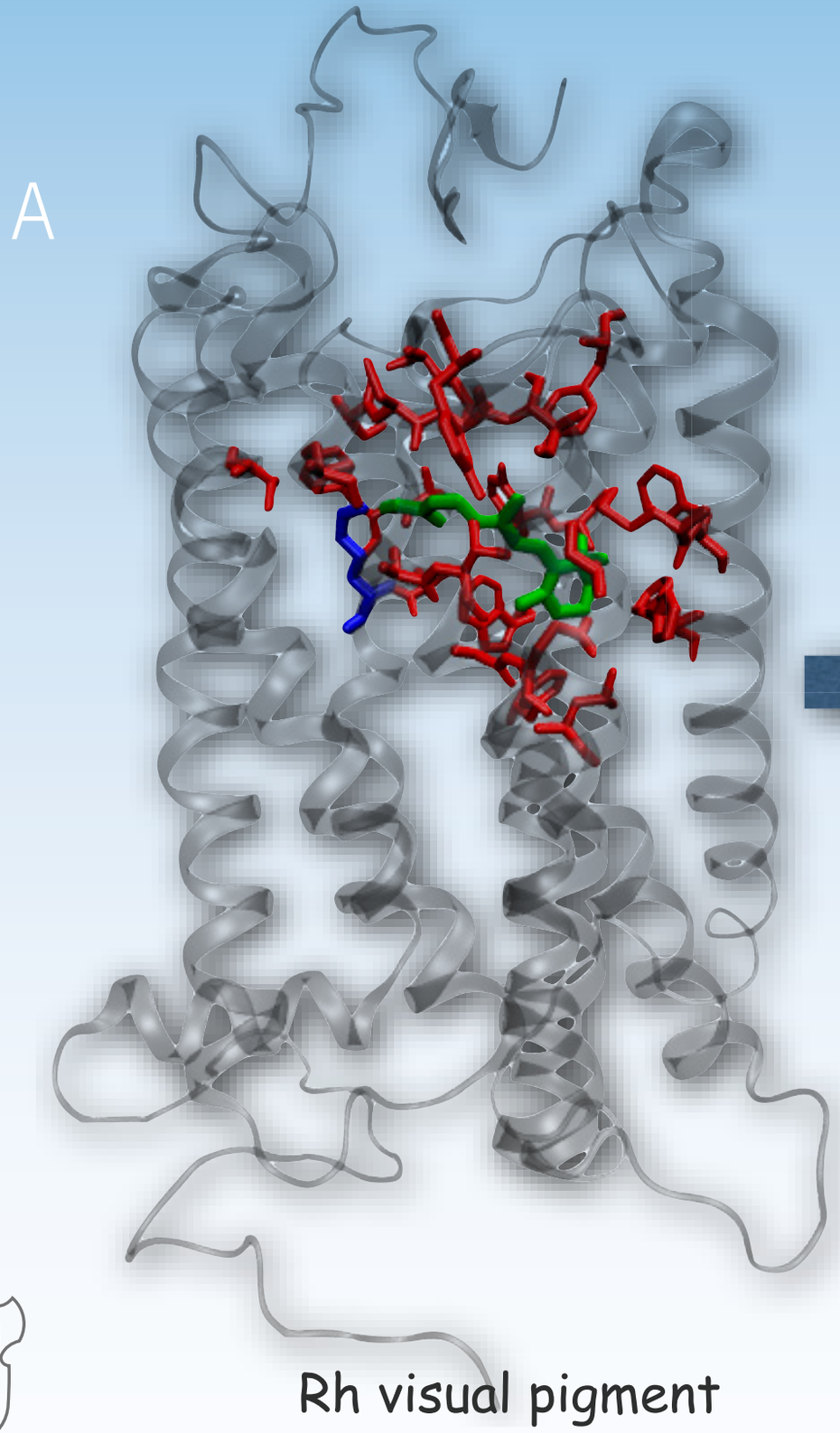
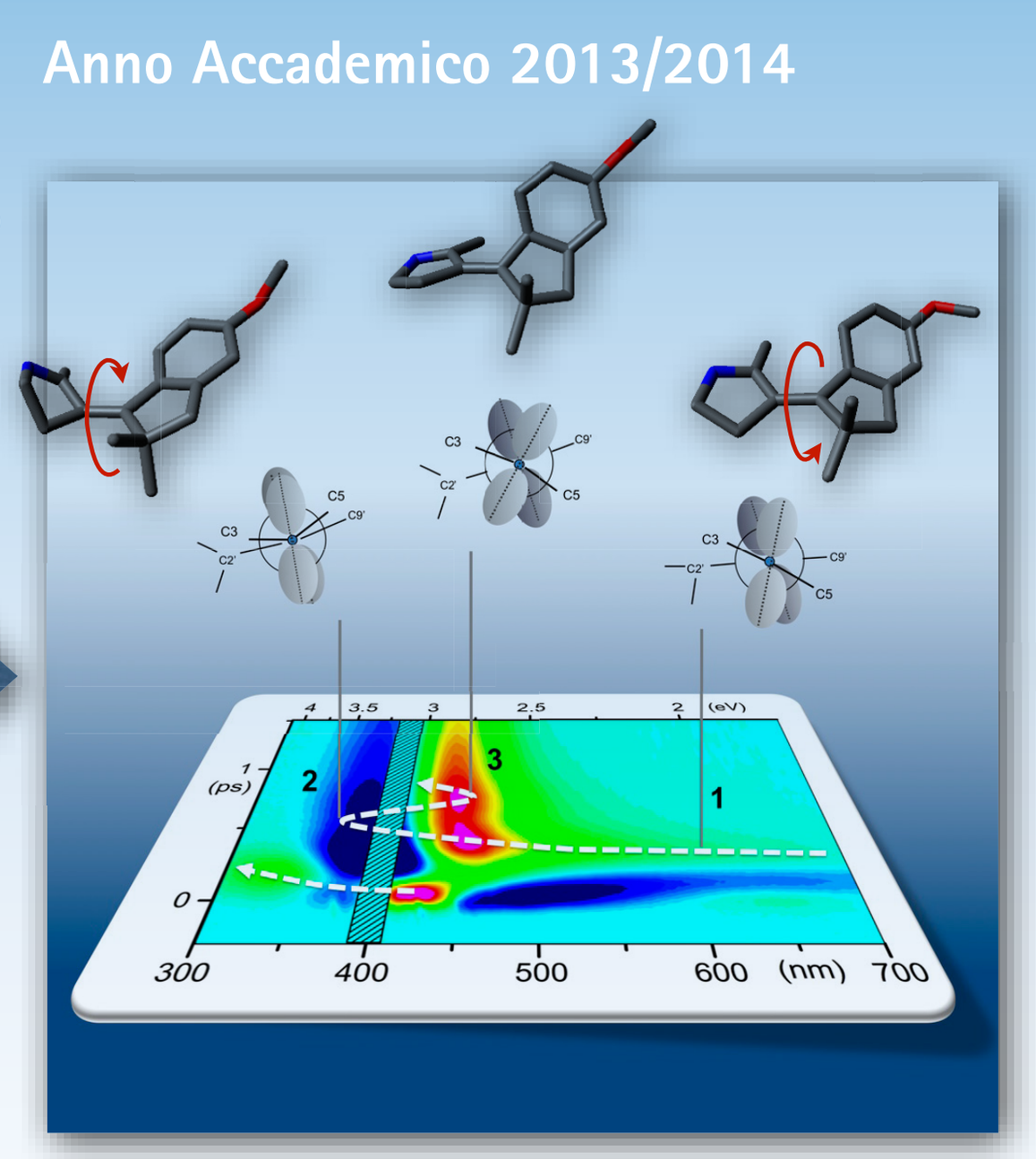
Mercoledì 18 dicembre 2013
Sala Stemmi
Palazzo della Carovana
Piazza dei Cavalieri
15.00

Colloqui della Classe di **Scienze**

Anno Accademico 2013/2014





coherent isomerization in a synthetic system

SCUOLA NORMALE SUPERIORE

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From Computational Photobiology to the Design of Vibrationally Coherent Molecular Devices and Motors

In the past multi-configurational quantum chemical computations coupled with molecular mechanics force fields have been employed to investigate spectroscopic, thermal and photochemical properties of visual pigments. Here we show how the same computational technology can nowadays be used to design, characterize and ultimately, prepare light-driven molecular switches which mimics the photophysics of the visual pigment rhodopsin (Rh) displayed in Figure A. When embedded in the protein cavity the chromophore of Rh undergoes an ultrafast and coherent photoisomerization. In order to design a synthetic chromophore displaying similar properties in common solvents, we recently focused on indanylidene-pyrroline (NAIP) systems. We found that these systems display light-induced ground state coherent vibrational (Figure B) motion similar to the one detected in Rh. Semi-classical trajectories provide a mechanistic description of the structural changes associated to the observed coherent motion which is shown to be ultimately due to periodic changes in the π-conjugation.

Info: Area Didattica - adi.sd@sns.it

Elaborazione a cura del Servizio Comunicazione e Relazioni Esterne | SNS