

Service des Photons, Atomes et Molécules
SÉMINAIRE

Mardi 15 mars 15h30

CEA-Saclay ;b; ;font color = 'red'; ;SPAM; /font; ;/b; Bât 522, p 138

Theory as a guidance for the interpretation and planning
of experiments

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A brief overview of the recent and current work of the Theoretical Chemistry Group at Rudjer Boskovic Institute will be given. The topics covered include quantum chemical modeling of the electronic and spectroscopic properties of hydrogen bonded systems, such as tunnelling splittings in the formic acid dimer, vibrational dynamics in microsolvated DNA oligomers and the Schiff base of n-butylretinal, as well as laser pulse control of population dynamics. Examples of reaction mechanisms of glycine oxidation by the OH radical in water and hydrogen storage in titanium doped sodium alanate will be given. In the second part, our studies in secondary structure formation in small model peptides and attempts at rationalizing their IR/UV spectra will be reviewed.

Le cafe sera servi 10 minutes avant

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http://iramis.cea.fr/Phocea/Vie_des_labos/Seminaires/index.php