ECAMP 15

Monday, June 30, 2025 - Friday, July 4, 2025

Book of Abstracts

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remains elusive. Analogous to magnetic effects induced by molecular rotation, twofold degenerate molecular vibrations, when excited with a $\pi/2$ phase shift, induce rotational motions of the nuclei, generating vibrational magnetic moments and intramolecular magnetic fields. We derive a consistent theoretical framework for these effective couplings, unifying nuclear spin-vibration and nuclear spin-rotation coupling. Calculations on benchmark molecules, which are known to show a vibrational Zeeman effect, demonstrate non-negligible vibrationally induced chemical shifts, and therefore a non-trivial intermolecular field geometry. Given the growing interest in molecular magnetism, particularly based on transition-metal complexes, we focus on metal phthalocyanines —a versatile, planar, macrocyclic molecules with a central metal ion —to identify configurations that maximize vibrationally induced magnetic effects.

#C7: Atomic and molecular spectroscopy, photo-induced processes

Highly oriented pyrolytic graphite chemical bonding structure after gallium implantation

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Highly oriented pyrolytic graphite (HOPG) structural changes caused by gallium (Ga) im-plantation at room temperature were investigated. To monitor structural changes in the sam-ples after implantation, Raman spectroscopy was used. SRIM (Stopping and Range of Ions in Matter 2013) software was applied to determine the depth profiles of Ga implanted at dif-ferent energies and the degree of damage in HOPG after implanting Ga. Accordingly, SRIM and Raman results suggest that amorphizing our HOPG sample requires a dpa above 4 dpa, which is much higher than previously reported (0.20 dpa).

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#C8: Atomic and molecular spectroscopy, photo-induced processes

Calculated absorption and circular dichroism spectra of TPPS4 molecular aggregates

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Recently there has been growing interest in TPPS4 for applications in photodynamic therapy as photosensibilizator [1]. The monomers of this porphyrin efficiently self-associate into H- and J-aggregates in aqueous media. It is not fully understood what kind of TPPS4 configurations are building blocks of molecular aggregates. For these reasons, the aim of this study is to determine tetramers and calculate their absorption and circular dichroism (CD) spectra.

First of all, quantum mechanical (QM) calculations were performed on geometry optimizations of the structures of TPPS4 zwitterionic monomers. Two different types of the zwitterionic form of the TPPS4 molecules were considered with respect to position of SO3H protonized groups: either these groups are opposite (Z1 monomer) or adjacent (Z2 monomer). QM calculation were performed using the DFT B3LYP/6-311G(d,p) basis set and polarizable continuum model (PCM) methods. The Gaussian 16 program was used. The next step was to take parameters from the General Amber force field (GAFF). It was also adjusted several parameters of monomers. Molecular mechanics (MM) geometry optimization was also performed. The second step was to construct Z1 and Z2 tetramers. The obtained tetramers were solvated with water boxes. Then molecular dynamics (MD) simulation was performed with AMBER 22 program.

Theoretical calculations of the TPPS4 tetramer's absorption and CD spectra were performed for Z1 and Z2 tetramers. The Frenkel excitonic model was used for this task as the electrons are localized to each molecule so we were able to treat each excitation as an exciton. These calculations were performed by associating 4 optical transitions to each molecule constituting the aggregate, which are in turn characterized by their respective transition energies for the Q and B band and an optical transition dipole moment vector for each transition (μ): i, j, k and l, the first two vectors corresponding to the Q band and vectors three and four to the B band. Each vector's coordinates were associated with the coordinates of each molecule's central nitrogen atoms. The tetramer's spectral density was calculated and then averaged for all 5000 frames of the simulation and normalized to a maximum of 1. It was determined two Z1 and Z2 linear tetramers. A comparison was performed of Z1 and Z2 tetramers absorption spectra with the measured spectra from the previous published article [2]. Our analysis of results demonstrates that larger peak shift of Z1 tetramer's spectra are more similar to the experimental data, however other configurations can be possible as well.

References
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#C9: Atomic and molecular spectroscopy, photo-induced processes

Atomic data for Os VI spectral lines of interest to nuclear fusion research from independent computational approaches

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It is now well established that the ITER Tokamak divertor will be made of tungsten (Z=74). During nuclear fusion operations, the divertor will endure some of the harshest conditions in the reactor. Thus, under neutron bombardment, tungsten will undergo nuclear transmutation, forming other elements, including osmium (Z=76). On the one hand, these impurities will contribute to the radiation losses and, on the other, they could allow to diagnose the fusion plasma in terms of impurity influx, temperature and density. Therefore, knowledge of the radiative data for Os ions is of great interest. The present work is focused on Os VI for which new transition probabilities were determined using two independent methods, namely the pseudo-relativistic Hartree-Fock including core-polarization effects (HFR+CPOL) and the fully relativistic Multiconfiguration Dirac-Hartree-Fock (MCDHF) ap-