ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ

ΤΜΗΜΑ ΦΥΣΙΚΗΣ

ΓΕΝΙΚΟ ΣΕΜΙΝΑΡΙΟ ΤΜΗΜΑΤΟΣ ΦΥΣΙΚΗΣ

PHYSICS COLLOQUIUM

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17:00 -18:00

3rd Floor Seminar Room

"Small-molecule endofullerenes: a quantum rotor in a box"

Dr. Toomas Rõõm

National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Abstract

Buckminsterfullerene C_{60} has a cavity large enough to hold a small molecule. Hydrogen is one of the few which has been incarcerated in the molecular cage of C_{60} and forms endohedral supramolecular complex H_2@C_{60}. Hydrogen acquires new properties because of confinement. Its translation energy becomes quantized and it is not free to rotate arbitrarily, and instead performs correlated translation and rotation motion. Because of the large mass difference of hydrogen and C_{60} and the high symmetry of C_{60} the problem is identical to a problem of a vibrating rotor moving in a three-dimensional spherical potential. The infrared activity of H_2 is induced by the translational motion within C_{60} cavity which breaks the inversion symmetry. We applied infrared spectroscopy to study dynamics of hydrogen isotopologs H_2, D_2 and HD incarcerated in C_{60}. Translation and rotation modes appear as sidebands to the hydrogen vibration mode in the mid infrared part of the absorption spectrum. The assignment of spectral lines to *para*- and *ortho*-H_2 was verified using *ortho* to *para* converted H_2@C_{60} sample. We derive dipole moment and potential parameters from the analysis of the infrared absorption spectra. H_2@C_{60} is a model system to test theories describing non-covalent interactions between molecular hydrogen and curved carbon nanosurfaces. Our results were used to develop pairwise additive five-dimensional potential energy surface for H_2@C_{60}. The same pairwise H_2-C_{60} potential that fits accurately infrared spectra of H_2@C_{60} was used to predict H_2 energies inside C_{70}. We compare the predicted energies and the infrared absorption spectra of H_2@C_{70}. Recently a water molecule was incarcerated in C_{60}. Water is a polar molecule and has a strong far-infrared response due to its rotation. We will show how the confining C_{60} affects the rotational spectra of H_2O at 4K and discuss the *ortho-para* conversion of H_2O at cryogenic temperatures.