Sažetak predavanja: „Squeezing hydrogen molecules in tight places: energetics, quantum dynamics, Raman, and inelastic neutron scattering spectroscopy“

Confining hydrogen molecules in nanoscale cavities leads to the quantization of their translational degrees of freedom, in addition to the quantized rotational states. This opens the door for the investigations of the quantum dynamics of coupled translational and rotational motions of the guest molecules, and how it is affected by the size, shape, symmetry, and chemical composition of the host cavity. We will review our rigorous treatment in the past couple of years of the quantum translation-rotation (T-R) dynamics of hydrogen molecules trapped in the small and large cages of the structure II clathrate hydrate and inside the fullerenes C_{60} and $C_{70,}$ and also in their open-cage derivatives. These studies have determined the maximum H_2 occupancy of the host cavities, and demonstrated the key role that the T-R zero-point energy plays in it. They have also have quantified the temperature dependence of the spatial distributions of the guest molecules, as well as their intricate T-R energy level structure exhibiting conspicuous patterns of degeneracies and level splittings. Quantum methodology for rigorous calculations of the inelastic neutron scattering (INS) spectra of nanoconfined molecules has been developed and implemented. Our findings are in excellent agreement with the recent spectroscopic measurements of these systems.