

Tailoring Functionality of Clusters and their Complexes with Biomolecules by Size, Structures and Lasers

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Absorption and emission properties of small silver clusters i) at surfaces and ii) in complexes with biomolecules based on first principle methods will be addressed in context of advanced optical data storage media and biosensing materials. Emissive properties require also determination of nonradiative lifetimes. It will be shown that this can be achieved by simulations of fs-pump-probe spectra based on nonadiabatic dynamics over conical intersections. Furthermore tailored laser fields will be used to drive photoisomerization processes in clusters and biomolecules. For this purpose new strategies for optimal control of i) pump-dump and ii) infrared processes in complex systems will be presented. Exploration and control of ultrafast dynamics is based on combination of quantum chemistry molecular dynamics (MD) "on the fly" and Wigner distribution approach.