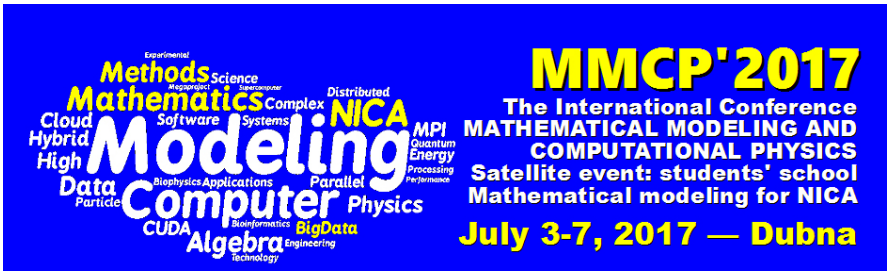

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ROADMAP FOR COMPUTER-AIDED MODELING OF THERANOSTICS AND RELATED NANOSYSTEMS.

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The key impact of nanotechnologies on many areas of research and development has become prominent in recent years. Biomedicine belongs to the most influenced fields by nanotechnology, for example thanks to the introduction of theranostics (systems for combined diagnostics and therapeutic utilization). These systems can be composed from metallic core nanoparticles functionalized with monolayer-covered bio-active molecules. Despite the recent "state of the art"level of molecular modeling methodologies and the number of articles published annually on noble-metal nanostructures, this particular field is still in discovery phase [1]. In addition, detailed understanding of interactions of such nanoparticles with biological membranes, macromolecules and other entities of the living cell has crucial importance for elucidation of the mechanisms governing biological actions of these nanosystems. Insights into molecular details how these nanomaterials interact with subcellular nano-machinery of the cells can facilitate design and engineering of new generation of nanoparticles [2]. We were interested in building and modeling thiolate-protected gold clusters and compute their static and dynamic properties, using our in-house hardware and software resources. In order to compare the performance issues for modeling of such complex nanosystems, we performed comprehensive testing of available software protocols.

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