The black ink dot at the very end of this sentence is about one million times larger than a typical quantum dot. Quantum dots are man-made semiconductor nanostructures; in other words—their sizes are on the order of one-billionth of a meter. Because of their unique properties, quantum dots are also known as artificial atoms. Thanks to recent technological progress it is now possible to embed quantum dots inside of nanowires. Nanowires are another kind of nanostructures. In fact, they are nanoscale whiskers with diameters thousand time smaller than an ant's leg. Since recently is it also possible to embed not only a single, but two quantum dots in a single nanowire. If a single quantum dot would be an artificial atom, then two or more of closely placed quantum dots should form an artificial quantum dot molecule, being a semiconductor counterpart of a real chemical molecule. Research on nanostructures is however not a simple display of nowadays technological marvels, but it allows for basic studies of matter and interacting systems. In particular, these works aim at understanding of how carrier charges interact with each other in systems where the particle movement in confined by nanoscale dimensions. Such research may have a large practical utilization for example in quantum communication, where the quantum character of light is used to protect against eavesdropping. Similarly there are advanced efforts on applications of quantum dots as quantum bits (qubits), forming a building blocks of future computers.

In the discussed project, while conducting theoretical and computational research, we aim to answer fundamental questions whether quantum dot molecule formed by two or three quantum dot can have a significant advantage over single quantum dots with respect to potential applications in quantum optics, cryptography and information.

We are interested in, among many, properties of electron-hole pairs, known as excitons, confined in these quantum dot molecules. Excitons emit light with particular spectral features and because of both practical and fundamental reasons it is important to understand detailed or fine structure of these spectra. Is it possible to control quantum dot molecular spectra with external electric field and utilize quantum dot molecules for entangled pair generation? Is alloy randomness and related disorder of atomic arrangement in quantum dot molecules causing so called dark, optically non-active exciton to gain some optical activity and no longer be of dark character? And how will this affect the opportunity of using the dark exciton as a quantum bit? Is a system of three quantum dots forming a quantum dot molecule and confining a triexciton a good candidate for a generation of entangled photon triplets?

We will try to answer these and many other challenging questions during the implementation of this project. This demanding task will involve utilization of complex computational methods. We will utilize an atomistic approach, where nanostructures are analysed atom-by-atom. In the project we will extend atomistic theory of nanostructures, by additional utilization of numerical methods used so far in astronomy and quantum chemistry. Many of computational results obtained during the project will involve complex analysis and access to high performance computers. In particular it might be immensely challenging to solve the so called inverse problem, for example to answer a following question: how to achieve certain spectral features by changing chemical composition or quantum dot shape in a quantum dot molecule? In order to solve the above task we plan to utilize machine learning approach, used typically in solving very complex problems related to artificial intelligence simulations. Results obtained in the project will have large practical meaning for researchers designing future nanostructures meeting certain functional traits. Besides applications in microelectronic or quantum information this research will also be important from a basic science point of view, for better understanding of spectral properties of confined many-body quantum systems.