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## MODELING THE EFFECT OF NANO MATERIALS ON BIOLOGICAL MOLECULE

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**M**olecular modeling is a class of computational work that depends mainly on quantum mechanical calculations. The detail of molecular composition and structures at the nanoscale is the first step to understand such systems which then produce the processes and control them. The challenges presented by nanoscience and nanotechnology are not simply restricted to the description of nanoscale systems and objects themselves, but extend to their design, synthesis, interaction with the macroscopic world, and ultimately large scale production. Another class of modeling application is to describe the biological interactions as

nanoscale materials enter to the biological systems. In this sense there are many experimental restrictions which gave the modeling work its priorities. In this sense the effect of nano metal oxides on the heme molecule is introduced as an example. Results indicate the possibility for nano metal to interact with heme molecule as a transition state and/or complex state which in turn could stop the action of heme molecule as gas transporter. The ability of interaction of some metal oxides is greater than those for O<sub>2</sub> and CO<sub>2</sub>.

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