

## PHYSICS AND ASTRONOMY COLLOQUIUM

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## "Towards First Principle Modeling of Biological Responses of Ionizing Radiation"

## <u>Abstract</u>

In this talk, I briefly review practical and computational approaches in modeling of the interaction of ionizing radiation with biological systems. Biological systems are exceptionally complex. In particular, cancer progression and treatment present several challenges that require multi-scale modeling. On the microscopic level, I present recent progress on large scale molecular simulations of initial damage of DNA-molecules interacting with randomly distributed clusters of diatomic OH-radicals, the primary products of megavoltage ionizing radiation. Physical and chemical pathways for carbonyl- and hydroxyl-hole formation in the sugarmoiety rings are identified. I show that gradual grow up of the holes lead to DNA-bases and DNA-backbone damages that collectively propagate to DNA single and double strand breaks. Possibilities in controlling and enhancing radiosensitivity via the application of nano-structures and developing dosimetry-based techniques for modeling radiobiological effects and biologically-guided radiotherapy (BGRT) relevant to the macroscopic level will be discussed. I conclude with remarks on possibilities for improving the biological metrics currently used in treatment plan validation and evaluation, and incorporation of the factors such as tumor surface morphology, fractal geometry, cancer cells invasiveness, hypoxic conditions and inclusion of the temporal and spatial correlations in the tumor control and normal tissue complexity probabilities that alter the radiation induced biological responses toward addressing the long term prognosis such as metastasis and second-cancer.

> Tuesday, March 31, 2015 3:00 p.m. Elliott Building Room 162