Multi-level Validation of a Nanodiamond Drug Delivery System, PSED Cluster 2009-2010

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Academic Disciplines:
MECHANICAL ENGINEERING
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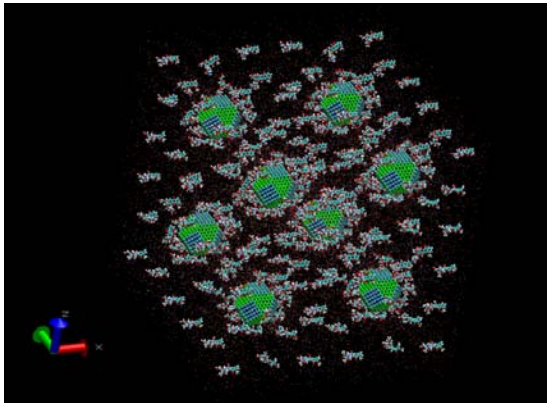
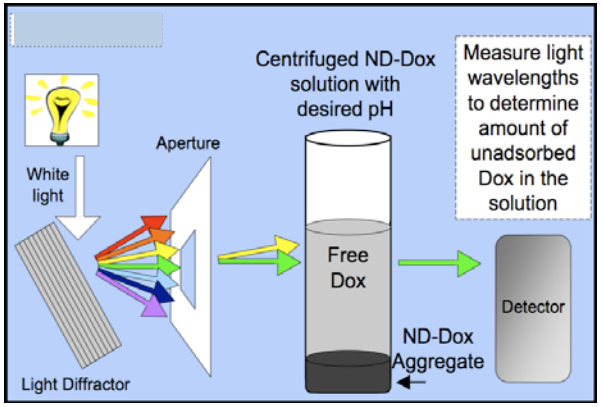
RESEARCH OBJECTIVE

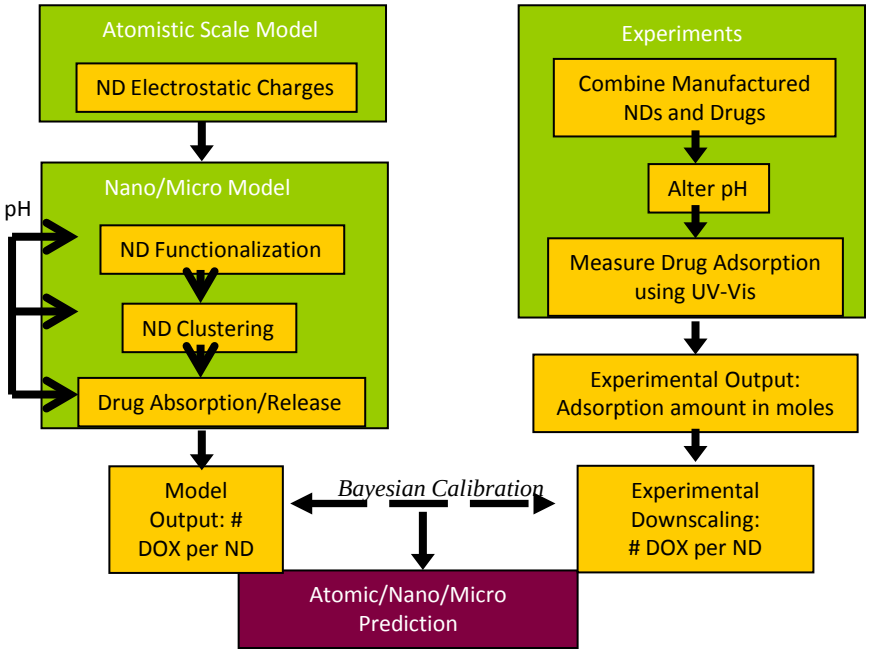
Collaborative effort to combine simulations and experiments at different physical scales in order to construct a predictive model for carbon nanoparticle (nanodiamond)-drug interactions. Bayesian calibration is required in order to bridge the differences between atomic/nanoscale simulations and micro-/mesocale experiments. Drug (doxorubicin) adsorption is simulated with varying amounts of carboxyl functional groups on the surface. Centrifugation pull-down and UV-Vis spectroscopy measurements confirm the amount of adsorbed drug onto nanoparticles in response to pH

SIMULATIONS

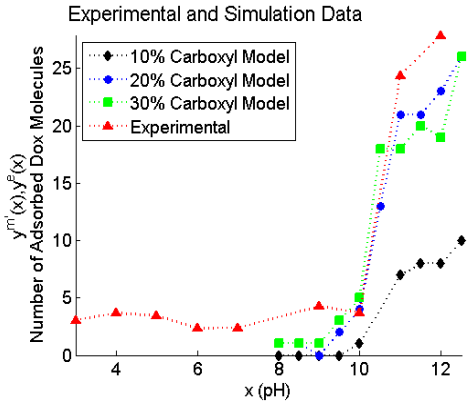


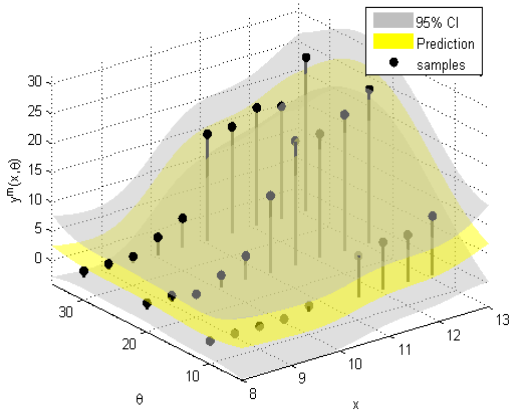
EXPERIMENTAL VALIDATION





COMPARISON AND FUTURE WORK





Resultant metamodels created from simulation and experimental data can be utilized to predict future nanodiamond-drug interactions, eliminating the need for costly comprehensive experiments and simulations.