Molecular Dynamic Modeling of Nanodiamond (ND) PEI Interaction Towards Delivery of Nucleic Acids

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Academic Disciplines:
MECHANICAL ENGINEERING, BIOMEDICAL ENGINEERING

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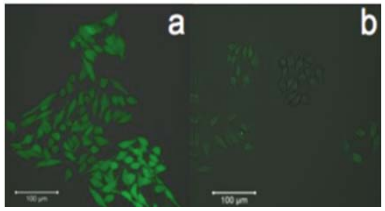
Motivation:

ND-PEI is a delivery platform capable of shuttling nucleic acids into cells in an in-vivo environment.

ND PEI combines the efficacy of industry standard transfection agents with superior biocompatability.



Research Need:

Use predictive science through modeling to inform the design of a more effective ND-PEI particle to delivery siRNA.

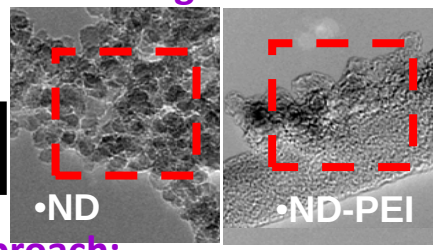
Future Work:

Incorporate siRNA into models.

Experimentally validate theoretical transfection efficiency of modeling-based particle design.

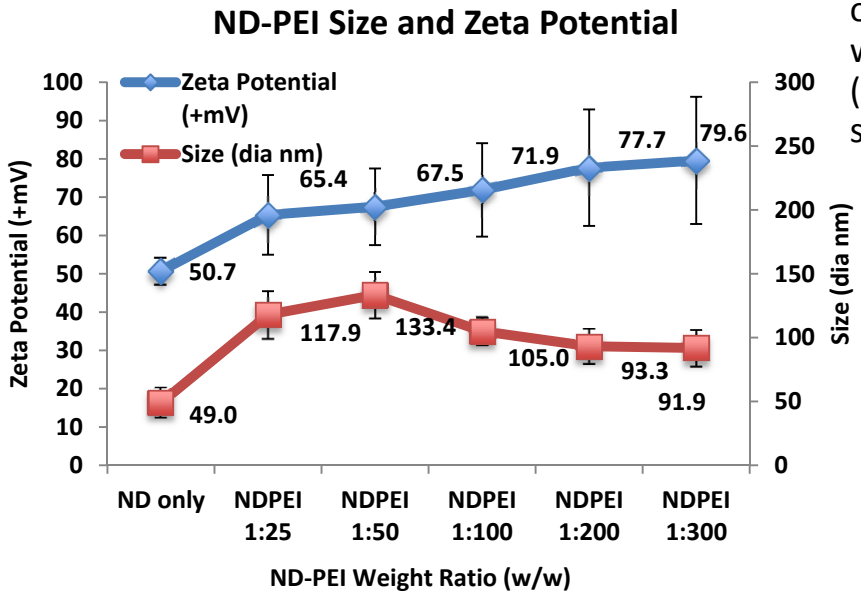
Goal: Understand the interaction between NDs and polyethylenimine (PEI) towards delivery of siRNA.

TEM Images:



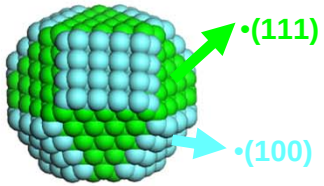
Experimental Approach:

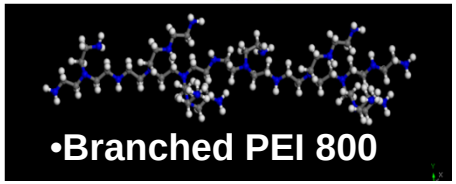
Measure the response of ND-PEI binding, with parameters of size and zeta potential, by varying pH and binding ratio of ND:PEI (w/w). Below is the sizing and zeta potential of particles with various binding ratios.

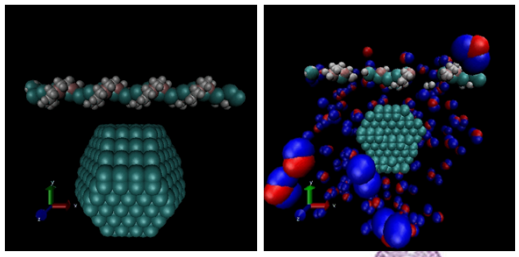


Modeling Approach:

Use molecular dynamics (MD) techniques to simulate the binding of ND and PEI in a solvent environment. Below is the model of the ND (top), and branched PEI (bottom) and the binding of PEI and ND with no solvent (left) and with solvent (right)







Conclusion: Shielding effects of water solvent reduces PEI loading

•Chen, M.; Zhang, X.-Q.; Man, H. B.; Lam, R.; Chow, E. K.; Ho, D. The Journal of Physical Chemistry Letters. 2010, 101019115841059-3171

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