

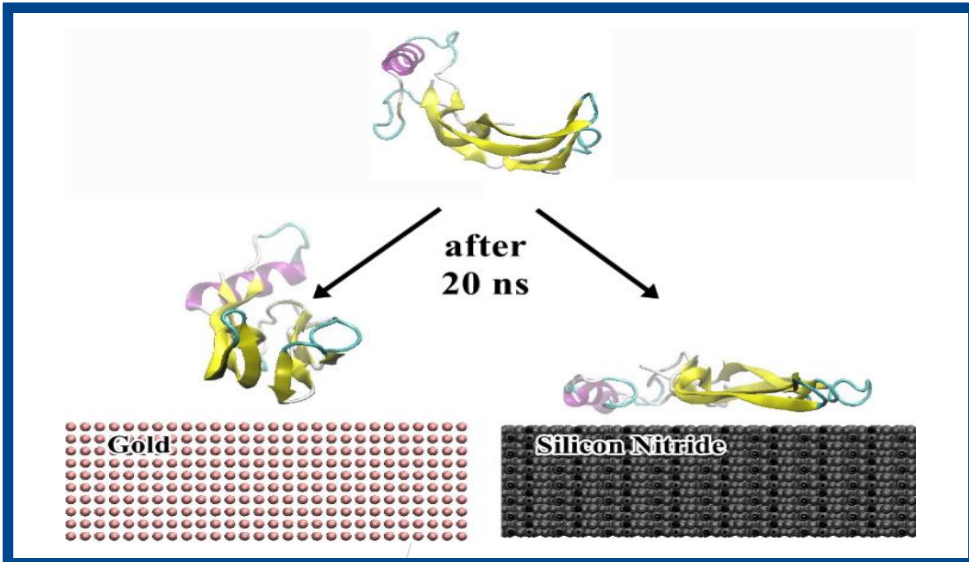


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*Program: Industrial and Systems  
Engineering*

*Dissertation Title: Understanding Multiscale  
Release Behavior of Biomolecules for Tissue  
Engineering*

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### RESEARCH QUESTIONS / PROBLEMS:

- Bone morphogenetic proteins (BMPs) are an important class of growth factors directly involved in many developmental processes for tissue and organ restoration. However, to obtain the desired repair of the tissues, the protein must be coated on material without any conformational changes that affect its bioactivity.

### METHODS:

- The interaction of BMP-2 with different substrates was studied using MD simulations were performed with NAMD and CHARMM force field. Simulations were performed for 0.2 ns of minimization and 20 ns of equilibration.

### RESULTS / FINDINGS:

- BMP-2 adsorption is a strong function of the three-way interaction between the protein, the dissolution media, and the substrate.
- Salt ions directly interfered with the adsorption process in the simulations performed with all substrates.

### SIGNIFICANCE / IMPLICATIONS:

- The protein adsorption process is highly dependent of the initial orientation of the protein. Silicon dioxide induces high conformational changes, causing protein denaturation.