**Investigating the Specificity of Peptide Adsorption on Gold Using Molecular Dynamics Simulations**

**Key Words:**

CHARMM22 force field, TIP3P model, Semiempirical embedded atom models, Lennard-Jones Potential, NAMD, Scalable Molecular Dynamics, visualization package VMD, Visual Molecular Dynamics

**Summary:**

Molecular dynamics simulations were performed on adsorption of gold-binding and non-gold-binding peptides on gold surfaces modeled with dispersive interactions. They performed simulations in three circumstances: peptides in solution, solvated peptides approaching a gold surface, and peptides approaching a gold surface in vacuum. All simulations are performed using the CHARMM22 force field for the peptides and buffering ions and the modified TIP3P (mTIP3P) model for water. They use the simulation package NAMD, Scalable Molecular Dynamics and the visualization package VMD, Visual Molecular Dynamics. Simulations are performed in either the NPT or the NVT ensembles at 310 K and a pressure of one atmosphere. Within the limitations of the approach, results indicate that when the peptides are solvated, adsorption requires both configurational changes and local flexibility of individual amino acids. This is achieved when peptides consist mostly of random coils or when their secondary structural motifs (helices, sheets) are short and connected by flexible hinges. In the absence of solvent, only affinity for the surface is required: mobility is not important. In combination, these results suggest the barrier to adsorption presented by displacement of water molecules requires conformational sampling enabled through mobility.