Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Investigating the specificity of adsorption of onto gold by gold-binding peptides using molecular dynamics simulations[1] ANA VILA VERDE, JANNA MARANAS, The Pennsylvania State University, Department of Chemical Engineering — It is possible to engineer artificial peptide sequences showing high specificity of adsorption for surfaces like gold, platinum or other solid materials. However, the reasons behind that high specificity are not clear. We investigate the adsorption of a genetically engineered peptide with high gold specificity using all-atom molecular dynamics simulations. Accurate Lennard-Jones parameters describing the interactions of gold with both water and amino acids are not currently available, so thus we discuss assignment of appropriate values. Two sets of simulations are presented: one using peptides made of a gold-binding motif (MHGKTQATSGTIQS) and another using peptides made of a non gold-binding motif (AIRRDVNCIGASMH). Adsorption onto the (111) and the (100) crystalline faces of gold is investigated. We discuss our results in light of the features of the peptide (sequence, charge, structure, nature of the amino acids) that may be responsible for the specificity of the gold-binding motif for gold.

[1]A. V. V acknowledges support from the Portuguese FCT through fellowship SFRH/BPD/20555/2004/0GVL

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Date submitted: 21 Nov 2006 Electronic form version 1.4