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Quantifying Polarization at Peptide-Gold Interfaces Due to Mirror Charges KSHITIJ JHA, HENDRIK HEINZ, Department of Polymer Engineering, University of Akron — The contribution of attractive polarization effects to interfacial interactions between even gold {111} and {100} surfaces with water, a neutral peptide (A3: AYSSGAPPMPPF), and a charged peptide (FlgNa_3: DYKDDDDK with Na counter-ions) in aqueous solution is quantified as part of an investigation to understand binding and specific interactions between peptides and metal nanoparticles. We apply the simple concept of mirror charges (additional Coulomb energy) a posteriori to molecular dynamics trajectories for different locations of the mirror plane, using the Consistent Valence Force Field (CVFF) extended with accurate LJ parameters for fcc metals. The values of polarization energy show a relative trend A3 < Flg-Na_3 < H_2O, and they are lower on {111} surfaces compared to {100} surfaces. On average, polarization energies amount to ∼140 mJ/m^2 when the image plane is located at the jellium edge and decrease to ∼5 mJ/m^2 when the image plane is located at the metal surface plane. Experiment and theory suggest a location close to the jellium edge, possibly inwards to the metal surface plane. Though absolute values are thus high, up to 2 kcal/mol per amino acid, they are <10% of the experimental value of 1400 mJ/$m^2$for gold-water interfacial tensions and <10% compared to the strongest adsorbing amino acids (>20 kcal/mol).

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