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Peptides at Aqueous Au and Ag Interfaces

Introduction

Interactions between biomolecules and materials interfaces are complex. Establishing a clear simulation can deliver a better understanding of the structure / property relationships governing the biotic / abiotic interface. The interactions between peptides and Au are of particular interest because of the wide range of applications, for example in materials synthesis, bio-sensing, and nano-medicine.

Method

GROMACS is used for all simulation, and Amber is used for force field. Before doing peptides at aqueous Au and Ag interfaces, we should establish a simple system that only contains water and interfaces without peptides. The following is the procedure. First Step, having a trajectory file of the interface, add water molecular into the system. Second Step, minimize the energy of the system, and check the structure of the interface and the potential energy of the system. Third Step, do NPT simulation for 2 ns to correct the water density. Berendsen and V-rescale method are used for pressure coupling and temperature coupling respectively. Semi-isotropic is set for pressure and the reference pressure is 1 bar. The reference temperature is 300 K. Final step, do NVT simulation for total 10 ns for production run. The temperature coupling method is set as same as in NPT simulation.

Results

After energy minimization, potential energy of the Au-water and Ag-water system is checked as shown in Fig. 1, and the structure of the interfaces and water molecular both looks like Fig. 2. In general, potential energy takes a value of 10 to power of 5 to 6. And we can see that both systems reach equilibrium. Fig. 3. shows that after NPT simulation, the pressure in z-direction fluctuates in a certain range, which means the system is stable.

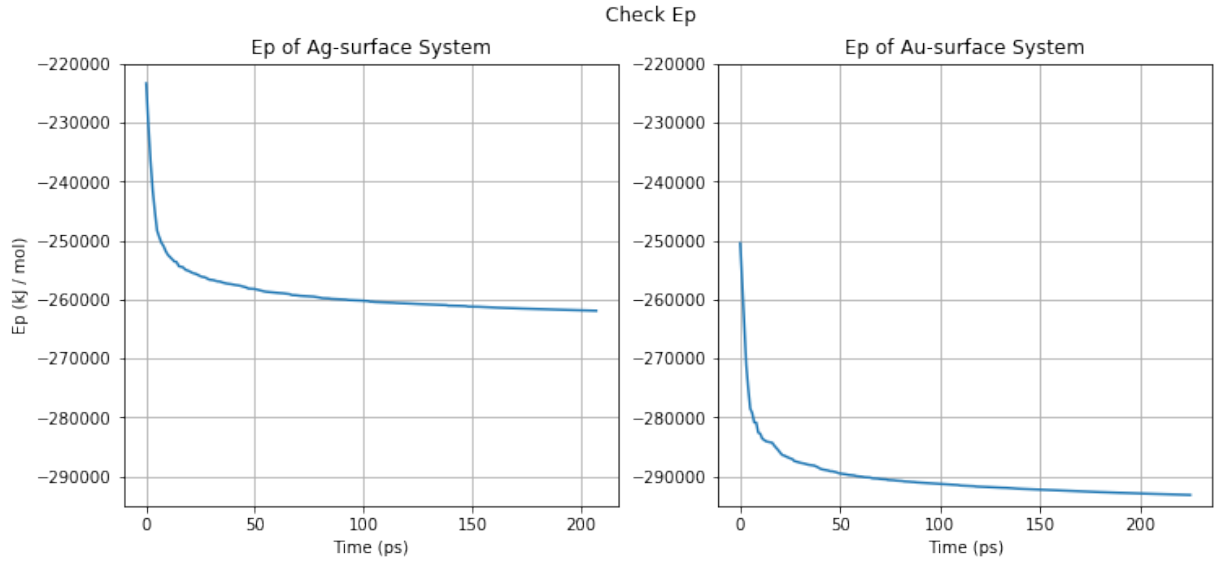

Fig. 1. Potential Energy of the System

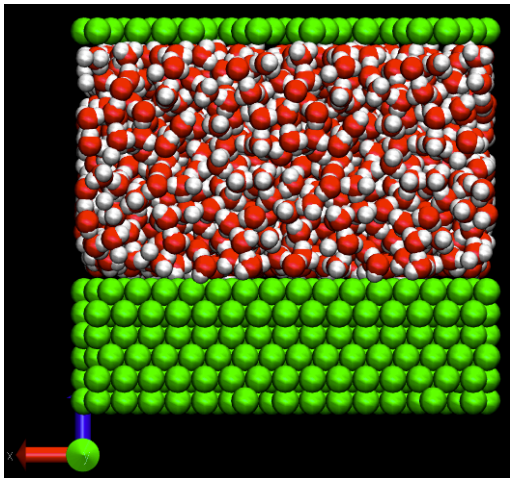

Fig. 2. The structure of the interface and water molecular

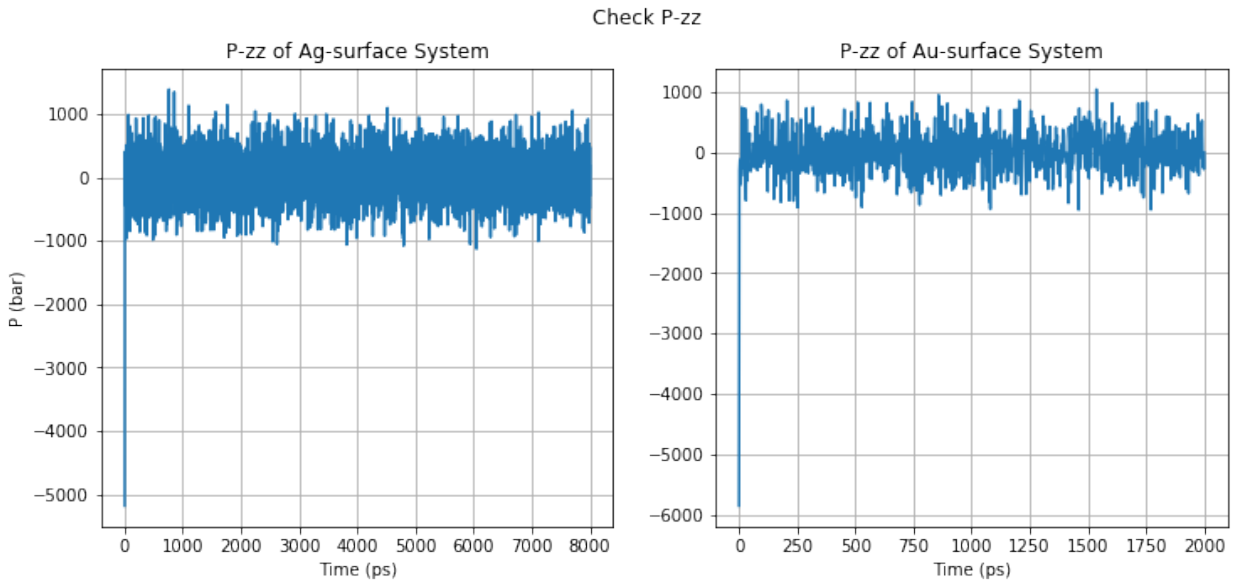

Fig. 3. Pressure in z-direction

After production run, we can calculate the distance between the water molecular and the surface, as shown in Fig. 4. In the calculation, a O atom represents a water molecular. We can see that before molecular dynamic simulation, the water molecular are randomly distributed. In contrast, after MD, there are two picks in the range of 0-0.5 nm and 2-2.5 nm, and the rest of the part remains the same, showing that the water molecular is attracted by the surface within about 0.5 nm. There are two interfaces because of the periodic condition, as shown in Fig. 2.

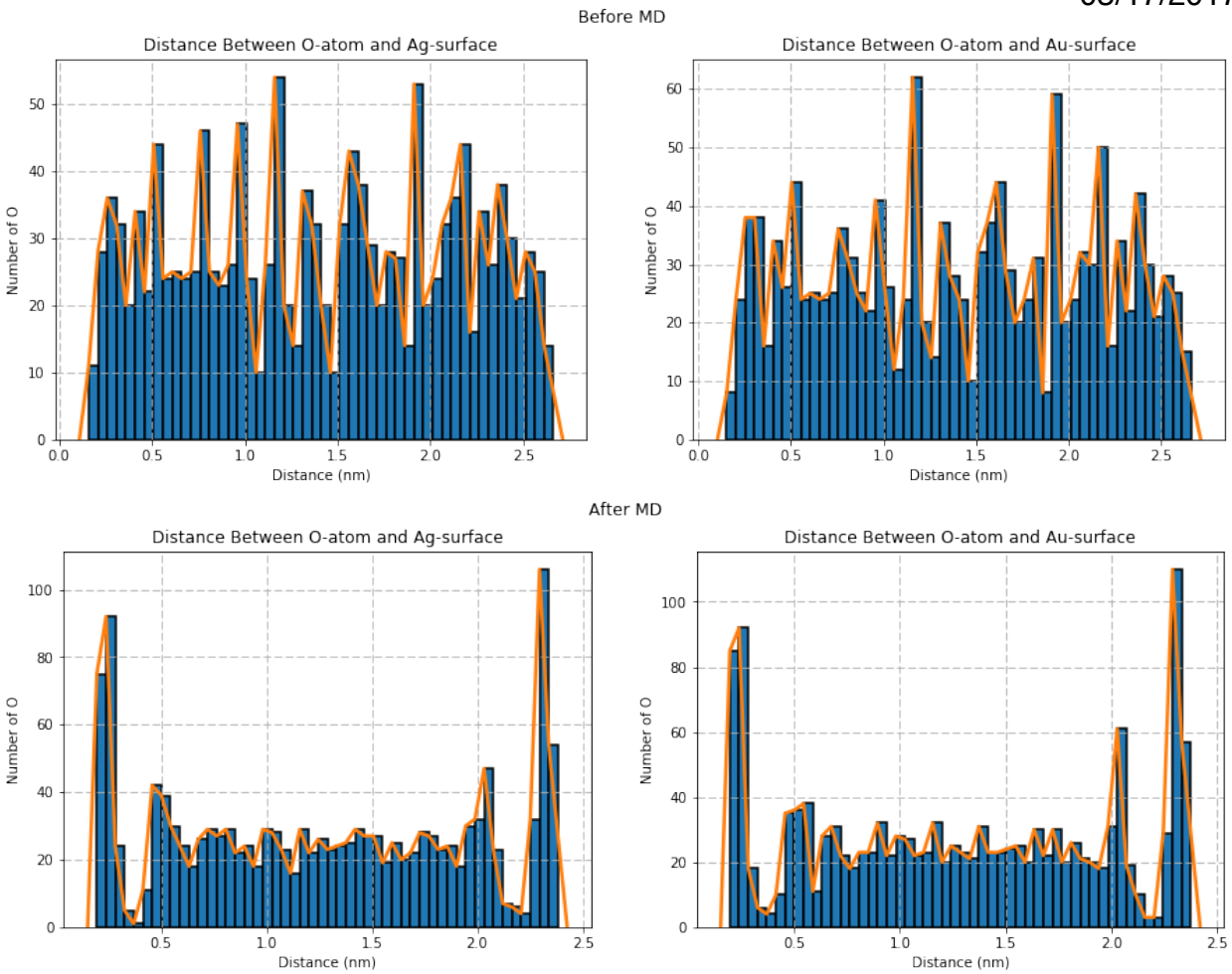

Fig. 4. A histogram showing the distance between the water molecular and the interface