QM/MM and classical MD simulation of His-tagged peptide immobilization on Ni surface

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The hybrid quantum mechanics (QM) and molecular mechanics (MM) method is employed to simulate the His-tagged peptide adsorption to ionized region of Ni surface. For simplicity, the peptide interaction with one Ni ion is considered. In the QM/MM calculation, main atoms around Ni ion are treated as QM part calculated by GAMESS, and the rest atoms are treated as MM part calculated by TINKER. The integrated Molecular Orbital/Molecular Mechanics (IMOMM) method is used to deal with the connection of QM and MM. By using QM/MM method, we calculate the binding energy of different possible structures, and the geometries data are also obtained. We also perform a classical molecular dynamics (MD) simulation for the synthetic peptide adsorption on neutral Ni(100) surface. We find that half of the His-tags are almost parallel with the substrate, which enhance the binding strength. Peeling of the peptide from the Ni substrate is simulated in the aqueous solvent and in vacuum, respectively. The critical peeling forces in the two environments are obtained. The results show that the imidazole rings are attached to the substrate more tightly than other bases in this peptide. And we trace the change of the typical structure of imidazole ring in all the process.

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