Water Molecular Adsorption on the Low-Index Pt Surface: A Density Functional Study

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Abstract	We report the different way to explain the nature of water molecule (H2O) adsorption on the platinum (Pt) surfaces with low Miller index, i.e., (100), (110) and (111). Here, we perform periodic density functional theory (DFT) calculations to analyze the correlation between water-surface bonding strength and the observed charge transfer occurring in the systems. The results show that Pt-H2O interaction strength at the most stable adsorption sites, i.e., the atop site for each surfaces, follows the order of H2O/Pt(110) > H2O/Pt(100) > H2O/Pt(111). This order has the same pattern with the order of observed charge transfer contributed to the bonding formation. The differences in adsorption geometrical structures in these three surfaces are suggested to responsible for the order of bond strength since Coulomb interaction plays dominant roles in our electrostatic model. Furthermore, H2O-Pt interaction mechanism, which occurs through water 3a(1) orbital releasing electron density (charge) followed by Pt-O bonding formation, is clarified.
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