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Water-Pd Interface in Catalytic Biomass Conversion: Atomic-Scale Structure and Properties YAKE WANG, SHUXIA YIN, XIN LIU, DARWIN SHIELDS, SANWU WANG, Department of Physics and Engineering Physics, The University of Tulsa — Biomass pyrolysis and other relevant catalytic reactions often occur at the liquid-solid interface. It is therefore of great importance to investigate the interfacial structure and other properties in order to achieve a deep understanding about the catalytic reactions for biomass conversion. We used *ab initio* molecular dynamics simulations to study the interfaces formed by liquid water and the palladium surfaces. Such interfaces are involved in many catalytic reactions for biomass conversion. We report results about the structural properties of the water/Pd(100) and water/Pd(111) interfaces, the interaction between liquid water and the metal surfaces, and how the interaction affects the structure. We found that while the interaction between water and the metal surface is weak, it could still cause considerable effects. In particular, the interaction promotes the formation of close-packed local clusters of liquid water.

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