

Abstract Submitted
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Importance of second neighborhood ensembles on PdAu bimetallic surfaces¹ DINGWANG YUAN, RUQIAN WU, XINGAO GONG — Atomic configurations of two or three Pd substituents on the Au(111) and Au(001) surface are investigated using the first-principles pseudopotential plane wave approach. Pd atoms are found to form second neighborhoods on PdAu surfaces. The Pd-d band becomes narrow and well below the Fermi level, very different from those in a Pd film or bulk Pd. Yet the surface Pd atoms are still active and serve as independent attractive centers towards adsorbates. Through studies of example reactions such as CO oxidation, ethylene dehydrogenation and vinyl acetate synthesis, we demonstrate the importance of special ensembles in catalyzing reactions by confining reactants in a small region.

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