

Abstract Submitted  
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**Role of electronic structure and surface structuring effects in the synergistic catalytic activity of Ni-Pd nanoparticles** LINN LEPPERT, Theoretical Physics IV, University of Bayreuth, 95440 Bayreuth, RHETT KEMPE, Inorganic Chemistry II, University of Bayreuth, 95440 Bayreuth, STEPHAN KUEMMEL, Theoretical Physics IV, University of Bayreuth, 95440 Bayreuth — Nickel-palladium nanoalloys show a drastically enhanced catalytic activity in a variety of hydrogenation reactions as compared to pure nickel or palladium nanoparticles. We explore the mixing behavior, electronic structure and magnetic properties of nickel-palladium clusters using density functional theory to gain insight into this synergistic effect. We show that the binding energy of hydrogen to the metal nanoparticle's surface, which can be tuned via the nickel-palladium composition, is the decisive factor determining how efficiently the reaction can take place. The optimal magnitude of the binding energy for intermediate nickel-palladium ratios can be traced back to a purely electronic effect: a balanced hybridization of the hydrogen  $s$  with the metal particle  $d$  and  $s$  states. This explanation not only holds for small clusters, but also for nickel-palladium surfaces. Finally, we demonstrate that catalytic activity on nickel-palladium surfaces might not only benefit from alloying, but also from the formation of nanostructures on surfaces.

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