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A DFT Study of the Interaction of Monometallic Pd_n/Pt_n (n=1, 9) Clusters with γ-Al_2O_3(100) Surfaces NALIN FERNANDO, New Mexico State University, Las Cruces, TYNE JOHNS, University of New Mexico, Albuquerque, YUE QI, CHANG KIM, General Motors Global R&D, Warren, MI, ABHAYA DATYE, University of New Mexico, Albuquerque, BORIS KIEFER, New Mexico State University, Las Cruces, NEW MEXICO STATE UNIVERSITY, LAS CRUCES COLLABORATION, UNIVERSITY OF NEW MEXICO, ALBUQUERQUE COLLABORATION, GENERAL MOTORS GLOBAL R&D, WARREN, MI COLLABORATION — The reduction of carbon monoxide and hydrocarbon emissions in advanced low temperature combustion engines has become more difficult for the advanced combustion systems in transportation sector. Exploration of effect of interface formation on the electronic properties of the existing platinum group materials may provide insight for the new material development that rivals platinum. In order to address the effects of the interface on the electronic properties of small Pd_n and Pt_n clusters (n=1-9) with a γ-Al_2O_3(100) support we have performed density-functional-theory (DFT) computations. The preliminary results suggest that the most favorable Pd_9 binding geometry is characterized by four Pd atoms binding to both Al and O surface atoms. The average Pd-O bond length across the interface is $\sim$ 2.2 Å, corroborating the formation of bonds. The preliminary analysis of the electronic density of states shows that the main electronic modifications occur at the Fermi energy, leading to an overall metallic behavior. We will discuss cluster size effects on the character of bonding across the interface, its stability, and electronic structure.

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