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Unraveling the Role of Metal-Support Interactions in Heterogeneous Catalysis

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We examine the role of the metal-support interaction in modulating the activity and selectivity of oxide-supported metal nanoparticles, focusing specifically on the Fischer-Tropsch (FT) synthesis of ethanol (EtOH). Although it is well-known that oxide supports can play a non-innocent role in heterogeneous catalysis, a comprehensive and predictive picture of the role of such supports remains elusive. Using realistic computational models of supported nanoparticles, we decouple the electronic and geometric aspects of the metal-support interaction, and we show that the former can be largely understood in terms of charge transfer between support and nanoparticle. The resulting metal-support interactions induce significant changes in adsorbate binding energies, and thus significantly influence reaction thermodynamics and kinetics. For the specific case of FT, we show how our model can be used to understand the observed increase in EtOH selectivity when switching from silica to titania supports. More generally, we illustrate how these ideas can be used to crudely predict the influence of a support even in the absence of detailed calculations and provide a general framework for understanding the influence of various oxide supports on elementary association / dissociation reactions.