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Decoupling the Effect of Pseudomorphic Strain and Electron Confinement on Catalytic Properties of Supported Metal Films RAJ GANESH PALA, FENG LIU, University of Utah — We present a model study of variations in reaction activation barriers as a function of thickness of a smooth metal film supported on a substrate. We demonstrate that the effect of pseudomorphic misfit strain and electron confinement can be completely decoupled by computing the adsorption-induced stress at the reactant's ground and transition state. This decoupling is based on linear elastic theory and is illustrated using first- principle calculations of CO dissociation on Ru film supported on the Os (0001) surface. The atomic coordination around the reactant is used to rationalize the nature of the adsorption-induced stress along the reaction coordinate. Furthermore, the effect of the different substrates (insulating/metallic) on the electron confinement is also addressed. The present model study will assist in making a quantitative estimate of the individual effects of misfit strain and electron confinement on chemical reactivity, thereby providing criteria for choosing catalytic metal films and their appropriate support.

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