

Abstract Submitted
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On relationship among composition, electronic structure and reactivity of catalytically active monolayers on metal substrates¹ SERGEY STOLBOV, SEBASTIAN ZULUAGA, University of Central Florida — Rational design of efficient electrocatalysts requires understanding of the relationship among the surface composition, its electronic structure, reactivity and catalytic activity. In this work by applying the first principle computational approach, we reveal the nature of the substrate effects on the electronic structure and reactivity of active monolayers (AM) deposited on a metal substrate (MS). In particular, we consider the Pt/MS structures (MS=Au, Ir, Ru, or Pt substrate). We reveal rationale for the interlayer hybridization to dominate over the strain effect in determining the AE/MS surface reactivity, in contrast to a widely accepted opinion that a strain is the main factor controlling the reactivity. We also find that, if AE is weakly bound to MS, the surface electronic structure does not suffice to characterize the surface reactivity, because of involvement of lattice response to adsorption of a reaction intermediate. We trace surface reactivity to a newly introduced hybridization parameter that reflects important features of the electronic structure of the AE/MS surface, which are not taken into account in the original *d*-band center model.

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