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The Effect of Structure Variations on Transition State Scaling Relations PHILIPP PLESSOW, SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering, Stanford University, Stanford, CA 94305, USA, FRANK ABILD-PEDERSEN, SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — Linear scaling relations for adsorption as well as transition state (TS) energies have proven extremely useful in the quest to identify, understand and predict reactivity trends of catalysts [1]. The existence of linear scaling relations for reaction intermediates can be understood in terms of simple bond order arguments and hence their accuracy depends on the variations in the adsorbate-surface bond [2]. Since structure and bonding of TS can vary substantially for different surfaces, it is much less clear that TS scaling relations should behave linearly at all. We investigated how the TS structure influences scaling relations and how scaling parameters relate to bond-orders. A model that accounts for varying geometry and goes beyond the linear approach is developed and applied to industrially relevant surface reactions.

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