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Title: Advances and Challenges in Computational Catalysis

Name: Grabow, Lars

Affiliation: University of Houston

Heterogeneous catalysis is widely considered as one of the key technologies for a sustainable and CO₂ neutral energy future, but new catalytic materials need to be discovered in order to achieve this goal. The field of computational catalysis on the basis of density functional theory (DFT) simulations has reached a level of maturity that not only improves our understanding of elementary reaction steps at the atomic scale,[1] but also allows us to propose materials with desired catalytic functionality.[2] Reactivity trends across transition metal catalysts can be explained in terms of the d-band model[3] and approximated by scaling[4] and/or Brønsted-Evans-Polanyi relations,[5] which enable us to rapidly screen for potential candidate materials. In this talk I will give an overview of the general strategies for computational catalyst design including notable examples from the recent literature. Shortcomings and possible improvements to the methodology will also be discussed. (1) Grabow, L. C.; Mavrikakis, M. ACS Catalysis 2011, 1, 365-384. (2) Grabow, L. C.; Studt, F.; Abild-Pedersen, F.; Petzold, V.; Kleis, J.; Bligaard, T.; Nørskov, J. K. Angewandte Chemie International Edition 2011, 50, 4601-4605. (3) Hammer, B.; Nørskov, J. K. Surface Science 1995, 343, 211-220. (4) Abild-Pedersen, F.; Greeley, J.; Studt, F.; Rossmeisl, J.; Munter, T. R.; Moses, P. G.; Skłason, E.; Bligaard, T.; Nørskov, J. K. Physical Review Letters 2007, 99, 16104-16105. (5) Wang, S.; Temel, B.; Shen, J.; Jones, G.; Grabow, L. C.; Studt, F.; Bligaard, T.; Abild-Pedersen, F.; Christensen, C. H.; Nørskov, J. K. Catalysis Letters 2010, 141, 370-373.