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Experimental modelling of "single-atom" catalysts: What defines molecular adsorption on single-metal sites?

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"Single-atom" catalysis (SAC) presents a recent frontier in catalysis research, promising to lower our dependence on precious metals and improve the economic viability of carbon-neutral technologies. Countless SACs were reported over the past decade, but rational design remains a challenge because the reactivity of "single atoms" is not easy to predict. The main hurdle is that the reactivity doesn't depend only on the metal atom used, but crucially also on the exact atomic-scale structure of its local environment. This renders many reactivity trends developed on nanoparticle catalysts inapplicable for SACs, and requires us to establish new descriptors that could guide efficient SAC research.

In my talk, I will show how we address this challenge from a surface science perspective. I will briefly outline the methodology, strengths and limitations of the surface science approach and I will demonstrate how it can be used to unravel the fundamental aspects defining molecular adsorption on model SACs. Specific focus will be placed on the interaction the "single-atoms" with the support, and how this can lead to stabilization of molecular adsorbates, specific reaction mechanisms or model catalyst deactivation.[1–5]

In our latest work, we strip away the support-dependent complexity by preparing the "single-atom" sites on surfaces that are chemically inert.[6] This allows us to mimic the active sites present in SACs based on N-doped carbon, and to assess their "intrinsic" reactivity.[7,8] We analyzed Fe^{2+} cations in various Fe-N_3 and Fe-N_4 geometries, and we demonstrate that even electronically identical sites can bind reactants with very different strengths.[8,9] These differences originate from distinct possibilities of structural relaxations, which cannot be predicted by analysis of electronic structure alone. Overall, these systematic studies unravel the fundamental aspects defining SAC reactivity, which is a critical prerequisite to rational SAC design.

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Date: Tuesday, April 28, 2026 - 4:15 p.m.
Lecture: Lecture Hall 05.01, ground floor, Universitaetsplatz 5, Institute of Physics, University of Graz
Host: Giovanni Zamborlini

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