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Surface scattering at extreme ultra-violet (XUV) free electron lasers

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The "Mobile Beamer surface scattering machine"is designed to make use of the advantageous properties of the radiation produced by the XUV free electron laser in Dalian[1] for surface scattering experiments on atoms and molecules. The XUV photolysis of small molecules will be used as a novel source of atomic beams, providing fine control over the electronic state and kinetic energy. In addition, the tunable XUV light source will be used for sensitive, isomer-specific detection of molecular scattering products and reaction intermediates at surfaces, via photoionization mass spectrometry with high time of flight as well as spatial and velocity map imaging resolution.

With this setup we would like to answer following three fundamental questions: Open-shell atoms can interact strongly with the electrons of a metal surface. For example, it has recently been shown that nonadiabatic "electronic friction" is the dominant energy dissipation mechanism that allows hydrogen atoms to stick to metals.[2]
1. To what extent do such forces govern the dynamics of heavier high-electron-affinity atoms (O, C, N) at surfaces? Will current theories for non-Born-Oppenheimer dynamics succeed in describing the scattering process of the atom?
2. Can electronic excitation of atoms lead to an increased reactivity with surface adsorbates or is the electronic energy lost to surface degrees of freedom without enhancing a reaction?

Although elementary kinetic models provide invaluable predictive power for gas-phase reactions, they are practically non-existent in surface chemistry due to the complex structure of interfaces. Recent work has provided the first transferrable kinetic model to treat the elementary site-specific processes in CO oxidation on platinum.[3]
3. By probing surface intermediates, can models based on elementary reaction steps be built for the predictive description of more complex catalytic systems?

[1] Deng Hai-Xiao et al., 2014 Chinese Phys. C 38 028101.
[2] O. Bünermann et al., 2015 Science 350 1346.
[3] J. Neugebohren et al., 2018 Nature 558 280.

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