CFEL SCIENCE

SEMINAR

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Building 99, Seminar Room I+II (EG)

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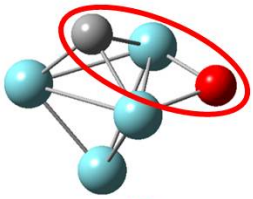
Molecular *versus* Dissociative CO Adsorption on Nb-Rh Nanoalloy Clusters

Cluster science provides an opportunity to tune the properties of clusters of one element by doping with other atoms. This additional dimension enables new questions to be posed such as whether the properties of the new cluster are intermediate to those of pure clusters of the elements involved. Here, the reactivity of CO with niobium-rhodium bimetallic clusters (or "nanoalloys") and their oxide counterparts in all three charge states have been investigated using a combination of Infrared Multiple Photon Dissociation (IRMPD) spectroscopy and Density Functional Theory (DFT) calculations. Experimentally, molecular adsorption of CO to various Nb-Rh nanoalloy clusters is indicated by the ion signal depletion of the pertinent carbonyl complex upon irradiation with IR light resonant with the C-O stretching frequency, ν(CO), of molecularly-bound CO. The absence of a *ν*(CO) band for a particular cluster is interpreted as CO being dissociatively-bound.

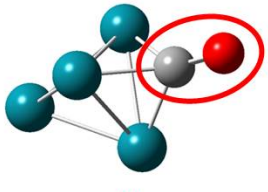
Overall, binding sites and interaction strengths have been characterised as a function of cluster size, composition (including O), and charge-state by observing how *ν*(CO) in the IRMPD spectra changes with these variables. Assignments have been made based on geometric information from DFT calculations. Additionally, reaction profiles constructed from various DFT-calculated minima and maxima provide detailed insight into the CO dissociation on bimetallic clusters, including C-O dissociation barriers, potential routes to facile CO dissociation, *etc*. The results of these recent experimental and computational investigations to date will be discussed in the presentation.



$Nb_4^{-/0/+}$ + CO
Dissociative chemisorption displayed in all three charge states.

$Nb_3Rh^{-/0/+}$ + CO?
$Nb_2Rh_2^{-/0/+}$ + CO?
$NbRh_3^{-/0/+}$ + CO?

Can the reactivity of CO be "tuned" with respect to the Nb:Rh composition ratio in nanoalloys? What about via sequential oxidation *i.e.*, $Nb_mRh_nO_x$ + CO?



$Rh_4^{-/0/+}$ + CO
Molecular chemisorption displayed in all three charge states.

Host: Melanie Schnell - CFEL Molecular Physics seminar