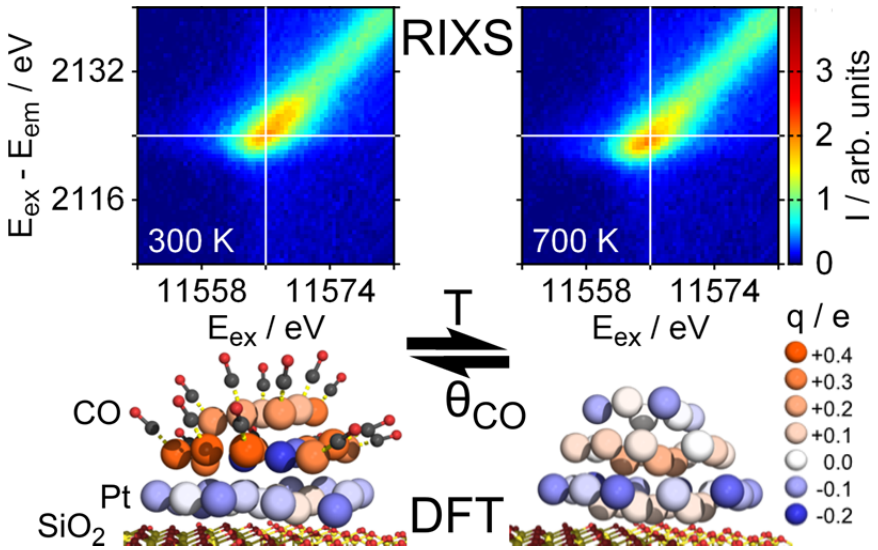
Intracluster atomic and electronic structural heterogeneities in supported nanoscale metal catalysts

This work reveals and quantifies the inherent intracluster heterogeneity in the atomic structure and charge distribution present in supported metal catalysts. The results demonstrate that these distributions are pronounced and strongly coupled to both structural and dynamic perturbations. They also serve to clarify the nature of the dynamic bonding of nanoscale catalytic metal clusters with their supports, and the mediation of these properties due to the presence of adsorbates. These findings are supported by theoretical modeling and experimental data measured for an exemplary supported metal catalyst, Pt supported on silica, using: *in-situ* high energy resolution X-ray absorption and emission spectroscopies; *in-situ* diffuse reflectance infrared Fourier transform spectroscopy; and *ex-situ* scanning transmission electron microscopy.

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