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Dynamic Structural Disorder in Supported Metal Nanoparticles: A Blessing or a Curse?

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Negative thermal expansion and anomalous bond length disorder are but a few examples of non-bulk behaviors in supported metal nanoparticles. I will illustrate them using a prototypical catalytic system, a platinum particle in equilibrium with oxide support and adsorbate gas, as an example. By combining X-ray absorption and emission spectroscopies with DFT/MD simulations, I will show that many "anomalies" have their explanation in the heterogeneous structure, fluctuating over broad time-scale. By tracking the flow of charge to and from the nanoparticle in operando conditions, several competing interactions can be disentangled: metal-support, metal-adsorbate, and support- adsorbate. In the ongoing research at Brookhaven our team is tackling also another type of heterogeneity, the inter-particle one, by creating a modern toolbox for operando investigations by a combination of spectroscopy and imaging methods. These results are of interest to energy sciences: by learning how to sort out and navigate these complex structures and employ dynamics to tune up reactivity, one can learn how to rationally design a catalyst with the desired activity and selectivity.