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The concept of localized atomic mobility: Unraveling properties of nanoparticles

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Nanoparticles (NPs) of transition metals have attracted much attention in the last decades because of their enhanced catalytic activities in different chemical reactions as compared to usual catalysts (e.g., transition-metal complexes or salts). The concept of short time scale mean-square displacement (MSD) was used to get a picture of the distribution of atomic mobilities in different layers and regions of Au and Pt NPs. The NPs were simulated in vacuum at different temperatures using molecular dynamics and the embedded-atom model. The calculated atomic mobilities were greater for atoms located at corner positions, followed by atoms on edges and planes, independently of the layer analyzed. The short time scale MSD was revealed to be an excellent alternative to predict melting temperatures of small (<100 atoms) transition-metal NPs. The combination of quantum and classical properties, namely, the d-band center with respect to the Fermi level and the short time scale MSD, respectively, has provided some insight into the understanding of how the catalytic activity may locally change over the NP surface. This methodology suggests that corner atoms are catalytically more active than those of edge or plane regions, which agrees well with the general idea that corner, kinks, and defect regions play a major role for the catalytic activity of metal surfaces. Also, size effects were observed here: upon decreasing the NP size from 1289 to 85 atoms, the NP surface has shown more pronounced differences between the atomic mobility of corner and edge regions. This suggests that local variations in the catalytic activity of a NP surface may become more dramatic upon decreasing the particle size, which stresses the importance of subnanometer-sized regimes for catalysis.

Keywords: Nanoparticles, Transition Metals, Phase Transition, Localized Atomic Mobility, d-Band Center