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Immobilizing Metal Nanoparticles on Single Wall Nanotubes. Effect of Surface Curvature.

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One to several nanometer-size nanoparticles possess supreme catalytic activity for a variety of important synthetic reactions compared to larger particles and bulk surfaces. However, a significant drawback is the catalyst durability as small, active, nanoparticles tend to merge to form larger, less active, nanocolloids. Tailoring the nanoparticle-surface support interaction could provide a means to limit nanoparticle mobility and thus prevent aggregation. In this study we demonstrate the stabilization of fine metal nanoparticles on nanotube surfaces by manipulation of surface curvature. Systematic density functional theory calculations of a large variety of nanoparticle-nanotube complexes revealed that the nanoparticle-nanotube binding interaction depends on, and can be controlled solely by, the surface curvature. Thus, an effective mechanism is demonstrated for the immobilization of small metal clusters with supreme catalytic activity on support surfaces. Furthermore, we provide experimental verification of our theory by comparing the aggregation of palladium nanoparticles decorating carbon nanotube and graphene surfaces as a function of time. Our theoretical predictions and experimental observations provide fundamental understanding to the physics of nanoparticle-support interaction and demonstrate how tailoring the support geometry can improve the durability of high performance nanocatalysts.

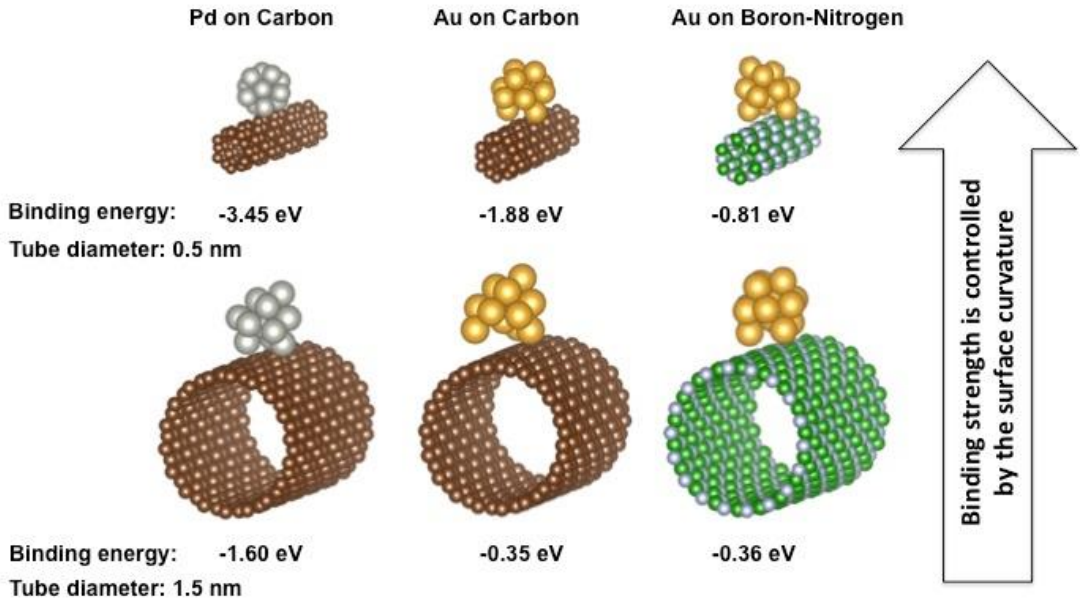

Figure 1: Binding interaction of ~1 nanometer metal particles can be controlled by the surface curvature. The particles bind strongly to curved surfaces and weakly to flat surfaces. The results are applicable to different metals, i.e., Au and Pd, as well as to different support surface, i.e., CNTs and BNNTs. The curvature of the support is responsible for the nanoparticle binding.