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Title:	Prospects in Engineering Congested Molecular Diffusion at the Stabilizer Layer of Metal Nanocrystals for Ultrahigh Catalytic Activity
Authors:	Sahoo, Lipipuspa (/jspui/browse?type=author&value=Sahoo%2C+Lipipuspa) Mondal, Sanjit (/jspui/browse?type=author&value=Mondal%2C+Sanjit) Garg, Reeya (/jspui/browse?type=author&value=Garg%2C+Reeya)
Keywords:	Palladium Molecules
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Abstract:	Electron transfer processes between a catalyst and a reactant molecule are inefficient beyond a couple of angstroms distance. However, the stabilizers of metal nanocrystals or ligands often create an outer shell that may extend beyond a few nanometers, which is considerably larger than the efficient electron-transfer length scales and suggests that the reactants must therefore diffuse through the shell toward the catalytic surface with a restrained diffusion rate to potentially slow the reaction. However, the effect of such diffusion behavior has so far been neglected as a contributing factor toward achieving high catalytic activities by noble metal nanocrystals. Herein, we examine this hypothesis using Pd nanocrystals having identical surface electronic structures but stabilized by shells of vinylpyrrolidone molecules in different fashions to show that (i) molecular diffusion near the catalyst surface can vary significantly and (ii) the diffusion barrier can improve severalfold, resulting in Pd nanocrystals exhibiting the highest turnover frequencies (TOF) reported to date for a variety of hydrogenation reactions, Suzuki–Miyaura cross-coupling reactions, and nitroarene reduction reactions. The work demonstrates the tailoring of the reactant diffusion barrier near the surface of a heterogeneous catalyst may offer new possibilities for improving the catalytic activity of noble metal nanocrystals.
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