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Title:	Understanding the role of solvent in determining the size and catalytic behaviour of Pd Nanocrystals
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Abstract:	<p>Solvents of synthesis can influence not only the size and shape of nanoparticles but also their catalytic properties. In an effort to understand the effect of solvents during the solvothermal synthesis of Pd nanocrystals (NCs), and the consequent effect in their catalytic properties, nearly monodispersed quasi-spherical nanoparticles have been synthesized by reduction of metal precursor salt H_2PdCl_4 using polyvinylpyrrolidone (PVP) as both reducing and capping agent in the solvent mixtures of water and ethylene glycol (H_2O-EG) in varying composition. Various characterization techniques such as transmission electron microscopy (TEM), powder X-ray diffraction (PXRD), Fourier transform infrared (FTIR) spectroscopy were utilized to explicate how methodical increase in the fraction of EG : 0%(v/v), 25%(v/v), 50%(v/v), 75% (v/v), 100%(v/v) in the mixture of H_2O-EG govern Pd NCs size and thus catalytically active surface area. The progression of Pd NCs size with an increasing fraction of EG shows a correspondence between the viscosity, boiling point, and dielectric constant of solvent and NCs size. This is also explained using Hansen solubility parameters which predicts solvent-mediated stability of capping agent around Pd nuclei during the growth step. Secondly, to gain insight into the influence of solvent used on Pd NCs catalytic activity, the above synthesized different sized Pd NCs efficiency is compared by carrying out Suzuki- Miyaura cross-coupling reaction and catalytic nitro-aromatic reduction reactions. A substantial difference observed in surface normalized turn over frequencies (TOF) and kinetic rate constants accentuate a deeper role of solvent beyond size control of NCs. This disparity in surface area normalized catalytic efficiencies is attributed to solvent-caused subtle differences in the surface energy due to factors such as different coverage density of capping agent PVP around Pd NCs, and the nature of surface atoms.</p>
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