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Essential role of strain in Photoluminescence of band gap engineered ZnO nanocrystals synthesized by low ARUP RAYCHAUDHURI, MANORANJAN GHOSH, S.N.Bose National Centre for Basic Sciences — The band gap of wide band gap semiconductor ZnO can be engineered by substituting (alloying) bivalent metals like Cd and Mg in place of Zn. We report synthesis of high quality nanocrystals of Mg and Cd substituted Zinc Oxide nano- crystals (8-10nm) and nanorods (length 25nm) by low temperature solution route. The substitution maintains the Wurzite structure. A continuous compaction of the lattice occurs when the Mg substitution takes place while there is a continuous expansion of the lattice on Cd substitution. This lattice compaction (expansion) blue shifts (red shifts) the band gap as well as the near band edge photo luminescence (PL) at room temperature. An analysis of the time resolved photoluminescence (TRPL) as well as the microstrain dependence of the PL line width suggests that in these nanoparticles there is excitonic localization by the random strain produced by the substitution. The investigation of optical and its correlation with structural properties indicate that in the band gap gets engineered mainly by strain.

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