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Fundamental Study on the Growth Mechanism of MoS_2 Quantum Dots: Impact of Reaction Time and Precursor Concentration

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Abstract : We aim to investigate the growth mechanism of molybdenum disulfide quantum dots (MoS_2 QDs) under hydrothermal reaction conditions by exploring two important parameters that control the growth process – (i) reaction time and (ii) precursor concentration. This fundamental study will focus on tuning the particle size, which eventually alters the optical and electronic properties of the QDs due to the quantum confinement effect, as well as monitoring the spatial growth of quantum dot sheets prepared through the aggregation of individual quantum dots. Among the mentioned two parameters, the former dictates the duration of aggregation while the latter controls the aggregation rate. The hydrothermally synthesized QDs have been analyzed through morphological and optical tools, and we used fractal analysis to understand the growth process. With increasing reaction time T (at a constant precursor concentration ≈ 73mM), the growth process shows a crossover from a bottom-up to a top-down process at T= 14 hours. A non-monotonic behavior of average QD size (d) is observed on the other side of it (d=7nm at T= 7 hours; d=16nm at T=14 hours; d=2nm at T=30 hours), which is supported by morphological studies like TEM and STEM, as well as optical studies like UV visible and PL spectra. Higher (lower) QD sizes correspond to lower (higher) bandgap and significant redshift (blueshift) in the PL spectra. The fractal dimension (f) of the QD clusters shows a sudden drop from 1.92 at this particular time T=14 to 1.82 and saturates at this value afterward. This signifies the onset of the fragmentation of the clusters due to the unavailability of active precursors. To validate the role of the precursors that have been claimed, we have carried out photophysical and statistical studies at a constant reaction time (14 hours) and have varied the precursor concentration instead. We observe a similar non-monotonic behavior in QD size (maximum size at ≈ 73mM) supported by the morphological and optical studies as the precursor concentration varies from 22mM (d=10nm) to 125mM (d=7nm). This is in agreement with fractal analysis, where the maximum df of 1.97 is observed at 73 mM which decreases at both higher (df = 1.67 at 125mM) and lower concentration (df = 1.75 at 22mM). This impact of precursor concentration is consistent for all reaction times. The fractal dimension of the QD sheets formed during the seeding and growth process is replicated for different reaction times as well as precursor concentration values through numerical simulations of random walk process on a 2D square lattice.

Keywords : aggregation and fragmentation, fractal analysis, optical studies, random walk
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