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Structure-based mechanistic insights into the biomineralization of CdS quantum dot

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Biomineralization is a control process in living organisms forming minerals from bioorganic molecules and inorganic solids. Bacterial biomineralization is an exciting area of research due to their inherent control over material growth from nanometer to the macroscopic level resulting multi-functional properties desirable for bioengineering and material engineering applications. Quantum dots (QD), also known as semiconductor nanocrystallites, are incredibly small particles ranging between 2 to 10 nm in diameter possess unique physico-chemical, opto-electronic and biological properties owing to quantum confinement effects. Semiconductor QDs have wide applications in fields ranging from display technologies, diagnostic imaging to solar cells. Furthermore, biosynthesis of QDs nanoparticle has several economic and environmental advantages over conventional synthesis, e.g. chemical based approaches that rely on high-temperature, often generates hazardous toxic wastes raising environmental safety and require expensive precursors. Here we present the crystal structure of an enzyme from S. maltophilia capable of aqueous phase synthesis of CdS nanocrystals QDs. The crystals are found to belonging to the orthorhombic space group , P212121 with unit cell parameters of a = 59.09 Å, b = 147.10 Å, c = 154.30 Å, α = β = γ = 90.00 ° and solved by molecular replacement method. This is the first crystal structure to our knowledge of an enzyme that is capable of both catalyzing the reactive precursors for mineralization and templating the subsequent nanocrystal growth. In the present study, crystal structures of apo and substrate bound forms are utilized to understand the mechanistic insights into structural determinants embedded in the sequence in the formation and growth of CdS nanocrystal QDs. Such understanding could provide clues to introduce novel protein engineering approaches to synthesize other quantum dots and open up new avenues for producing de novo design nanocrystals utilizing artificial protein units as a building block.

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