

**Title: A Computational Study on the Effect of Surface Passivation of PbSe and PbS Quantum Dots with Chlorine and Oxygen in various forms**

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PbSe and PbS quantum dots (QDs) are well known for their promising applications in a wide range of optoelectronic devices, including solar cells, light emitting diodes and lasers. Nevertheless the downside is that these materials are easily susceptible to oxidation that affects their optical and electronic properties. Thus it is intriguing to study the reason behind these affects and finding a solution to overcome this problem. Here in, we provide a DFT based computational methodology that shows some interesting results, through which experimentalists can understand the effect of surface passivation of various forms of chlorine and oxygen ligands that can enhance or decline the stability of QDs. We show how passivation increases or decreases the band gap and surface trap states; and improve photoluminescence efficiency.