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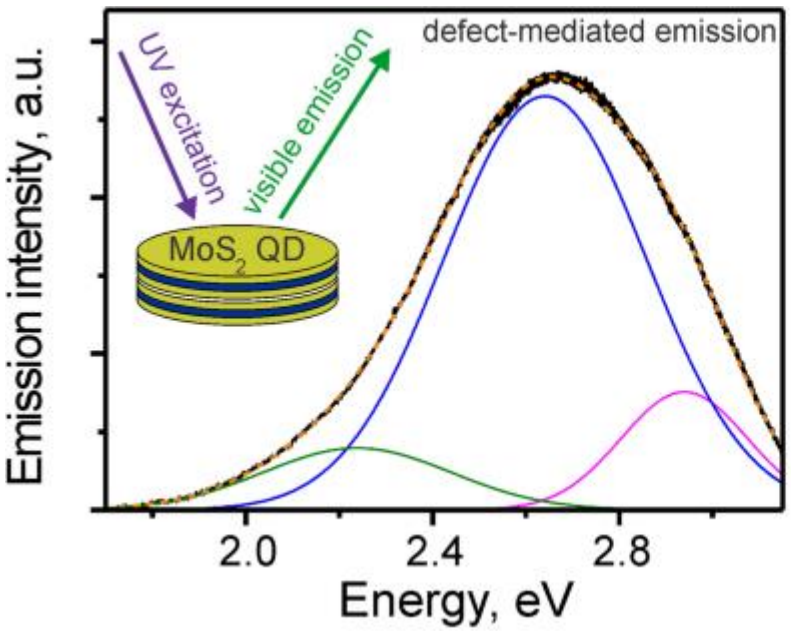
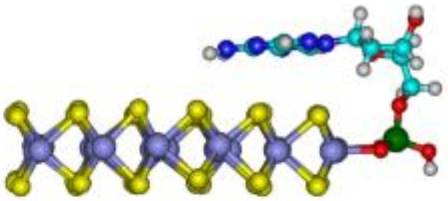
Abstract

In recent years, the use of biomolecules as dispersants for the preparation of 2D nanomaterials by direct liquid-phase exfoliation (LPE) using ultrasonication has attracted increasing attention as a convenient and cost-effective approach to ensure simultaneously the biocompatibility of these nanostructures. In this work, we prepare MoS_2 quantum dots (QDs) by the LPE method using deoxyadenosine monophosphate (dAMP) as an exfoliation agent that provides a good biocompatibility of the QDs too. As a result, a visible-range photoluminescence from MoS_2 QDs surrounded by nucleotides is observed for the first time. Different structures of MoS_2 QDs with dAMP are analyzed employing the DFT calculations. It is shown that dAMP can form coordination bonds with the Mo atoms located at the QD edges or at the defect sites where direct contacts with these atoms can occur. The covalent bonds facilitate strong adsorption of dAMP on a MoS_2 QD. The structural flexibility of the nucleotide adsorbed on the MoS_2 QD enables a combination of noncovalent stacking interaction of the nucleobase and a coordination bond of the phosphate group with the Mo atoms located at the edges to occur. This leads to the formation of a very energetically stable complex.

Graphical abstract





Binding of dAMP to edge or defect site: DFT calculation