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Photoluminescent MoS₂ quantum dots surrounded by nucleotides

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In this work, we have successfully dispersed MoS₂ in aqueous solutions of canonical nucleotides (dAMP, or dGMP, or dCMP, or UMP) by ultrasound-assisted exfoliation. We report the first observation of visible-range photoluminescence (PL) registered from all suspensions, which we attribute to the presence of MoS₂ quantum dots (QDs) in the suspensions. The comparison of PL band intensity, peak position, and spectral width suggests the essential role of MoS₂-nucleic base interaction for MoS₂ QDs exfoliation, colloidal stabilization, and the production of emissive quantum dots. Different structures of MoS₂ 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 MoS₂ QD. The structural flexibility of the nucleotide adsorbed on the MoS₂ 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.

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