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Binding mechanism of CdSe quantum dots to carbon nanotubes/graphene JIE JIANG, SOHRAB ISMAIL-BEIGI , Applied Physics, Yale University — Decorating carbon nanotube or graphene with CdSe quantum dots (QDs) is one approach to creating next generation high efficiency photovoltaics. We have used first principles methods to calculate the binding mechanisms of oleic acid (OA) to CdSe QDs as well as how -COOH functional groups can link the QD to graphene. In both cases, the strongest binding involves the terminating double-bonded oxygen atom in the -COOH group covalently bonding to a surface Cd atom while the hydrogen (from the OH part of the -COOH) aligns to make a weak hydrogen-like bond to a neighboring surface Se. We find a strong defect enhanced binding of the QD to graphene via -COOH: when the -COOH links the QD to a defect site on the graphene, the binding energy of the complex is 0.5 eV larger than when a -COOH links the QD to a pristine graphene region. These results are consistent with available edge X-ray absorption fine structure (EXAFS) data and also rationalize the growth procedure by which ultrasonication of the OA functionalized QDs leads to the replacement of some QD-OA bonds by QD-COOH-graphene bonds, which strongly link the QDs to the graphene surface.

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