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Construction of Symmetry-adapted k.p Hamiltonians for semiconductor nanostructures

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Using ab-initio methods like DFT for nanostructures is computationally very expensive, even with modern supercomputers. However, we will show that an accurate quantitative picture can be obtained with a k.p method by starting with Kohn-Sham (KS) states obtained from ab-initio calculations for bulk structure. We demonstrate this by comparing k.p with DFT calculations for the case of CdSe quantum wells. We obtain the analytical form and numerical parameters of well-studied 4x4 and 8x8 k.p Hamiltonians found in literature, for the case where spin-orbit coupling is omitted and included, respectively. Also, we demonstrate an improvement over 4x4 and 8x8 Hamiltonians, by expanding the number of states from 4(8) to 13(26), which yields more accurate excited states. Another improvement can be made, by using the GW approximation within the many-body perturbation theory, thus correcting the DFT electronic structure. This method can give more accurate bulk band gaps, which in turn yields improved results for nanostructures.