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Construction of symmetry adapted $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian from DFT calculations

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Electronic structure of semiconductors and their nanostructures can be described using the well known $\mathbf{k} \cdot \mathbf{p}$ perturbation theory of Kane for bulk materials and Burt for heterostructures. Corresponding Hamiltonians are represented in a basis of Bloch wave-functions and parameters of the Hamiltonian are related to momentum matrix elements between the basis states. Due to crystal symmetry some of these matrix elements vanish, while some have the same value and consequently the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian has a relatively simple form with a limited number of parameters. However, there is still no automatic way to obtain the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian in this standard symmetrical form from ab-initio electronic structure calculation. In this work, we established the procedure to achieve this. The first step of the procedure is to perform density functional theory calculation of material band structure and obtain the Kohn-Sham wave-functions. Next, for each of these wave-functions we determine the corresponding irreducible representation of the symmetry group and transform them to a standard symmetry-adapted basis. We then calculate the momentum matrix elements in this basis which leads to the parameters of desired $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. We illustrate the method by applying it to cubic lead-based perovskite $CsPbBr_3$ as seen in Figure below.

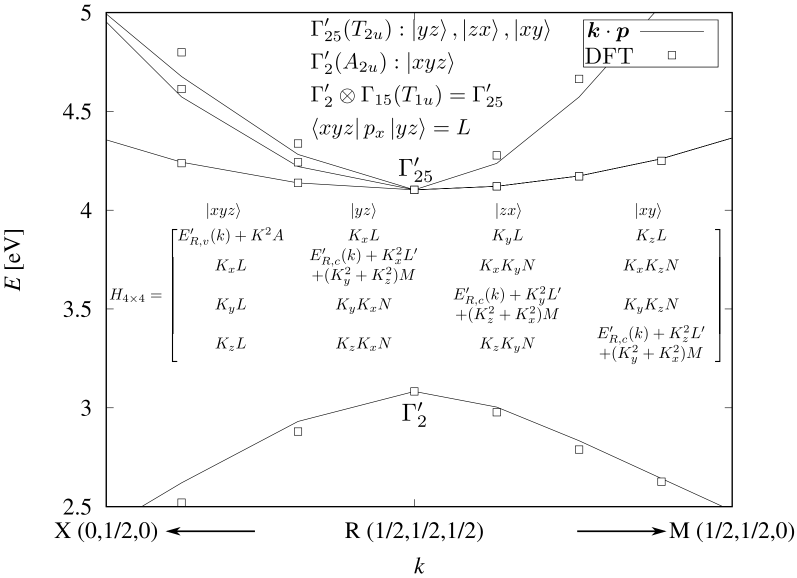

Figure 7: Calculated band structure of $CsPbBr_3$ near the band-gap (point R) obtained from DFT (squares) and from symmetry-adapted $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian (full line). Valence and conduction states at R correspond to irreducible representations Γ'_2 and Γ'_{25} , respectively. Alternative labels for irreducible representations, their partners and their product as well as an example of momentum matrix element are shown in the top inset. The symmetry-adapted $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian is shown in the bottom inset.