README:

About:

MATLAB codes of Slater-Koster formalism based tight-binding model designed for halide double perovskites. The codes contain tight-binding method to calculate the band structures. The model has been fitted to multiple compounds in the whole Brillouin zone, and the corresponding hopping parameters are also provided. We have also implemented the spin-orbit coupling effect in our model Hamiltonian. In addition, we have calculated the optical properties such as the momentum matrix element, the joint density of states, imaginary part of the dielectric constant.

The codes are also capable of calculating the electronic structure and optical properties of cation intermixed halide double perovskites. We have shown the example for $Cs_2AgIn_{1-x}Bi_xCl_6$ and $Cs_2Ag_{1-x}Na_xInCl_6$.

Requirements:

You need to have MATLAB software installed in your system.

Uses:

We have provided the step-by-step procedure in the comment lines of each code. The package contains the following folders.

(1) **TB_bands:** This folder contains the TB fitted band structures of 14 HDPs along with the fitted TB hoppings. There are three .m files in this folder; (i) **band_plot_dp.m**: This code has model Hamiltonian for $Cs_2AgBiCl_6$, $Cs_2AgInCl_6$, $Cs_2AgSbCl_6$, and $Cs_2AgTlCl_6$. (ii) **band_plot_pp.m**: This code has model Hamiltonian for $Cs_2InBiCl_6$, $Cs_2InSbCl_6$, $Cs_2TlBiCl_6$, and $Cs_2TlSbCl_6$, $Cs_2TlBiBr_6$, and $Cs_2TlSbBr_6$. (iii) **band_with_halide_p_orbitals.m**: This code contains the TB model Hamiltonian for $Cs_2NaInCl_6$, $Cs_2NaBiCl_6$, Cs_2KInCl_6, and Cs_2KBiCl_6. Here, Cl-p orbitals are also considered as the basis set to construct the Hamiltonian.

(2) **MME**: Plot the momentum matrix element (MME) along the high symmetry path of the band structure for the HDPs given in the TB_bands folder.

(3) **JDOS:** Plot the joint density of states (JDOS) for the HDPs given in the TB_bands folder.

(4) **Mixed_cation:** Calculate the TB band structure, MME, and JDOS for cation intermixed HDPs.

(5) **Hamiltonians:** This folder contains all the SK-TB Hamiltonians and SOC Hamiltonian.

(6) **DFT_data:** This folder contains DFT band eigenvalues and k-points.

(7) **DFT_bands_with_orbital_characters:** This folder contains the code to plot the DFT band structure with orbital characters.

N.B.

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