Supplementary Materials

Investigation into the Exciton Binding Energy of Carbon Nitrides on Band Structure and Carrier Concentration through the Photoluminescence Effect

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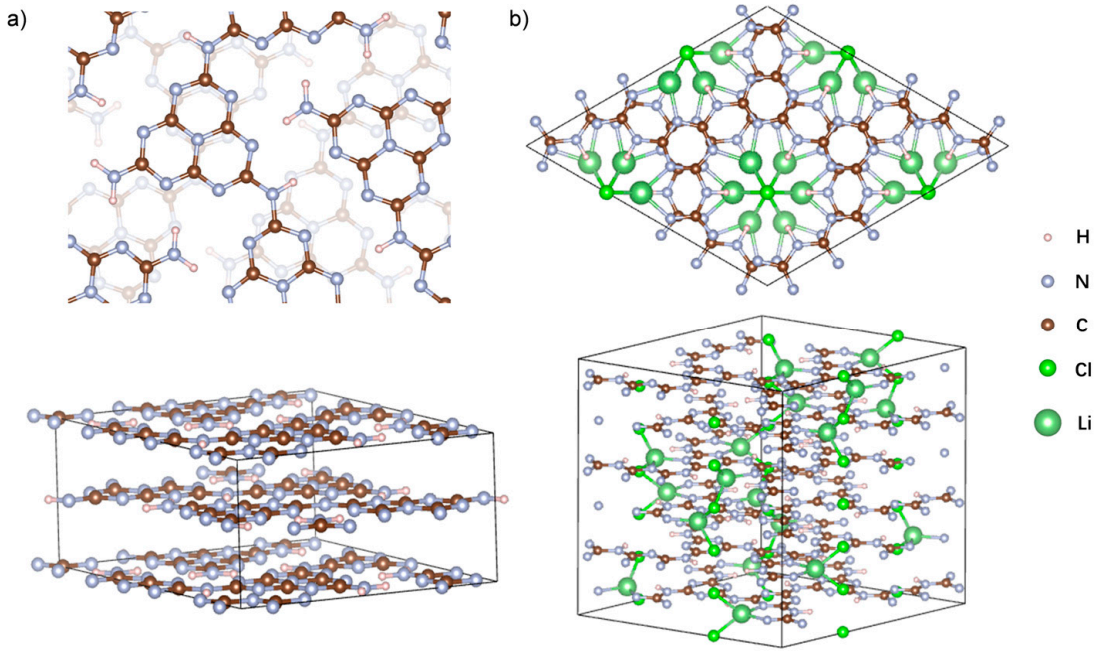

Figure S1. Structural basis applied for computation, a) ab stacking structure of melon b) the complete equal distribution of Li ions in each possible occupation site in the six-layer PTI/$Li^{+}Cl^{-}$ mode.

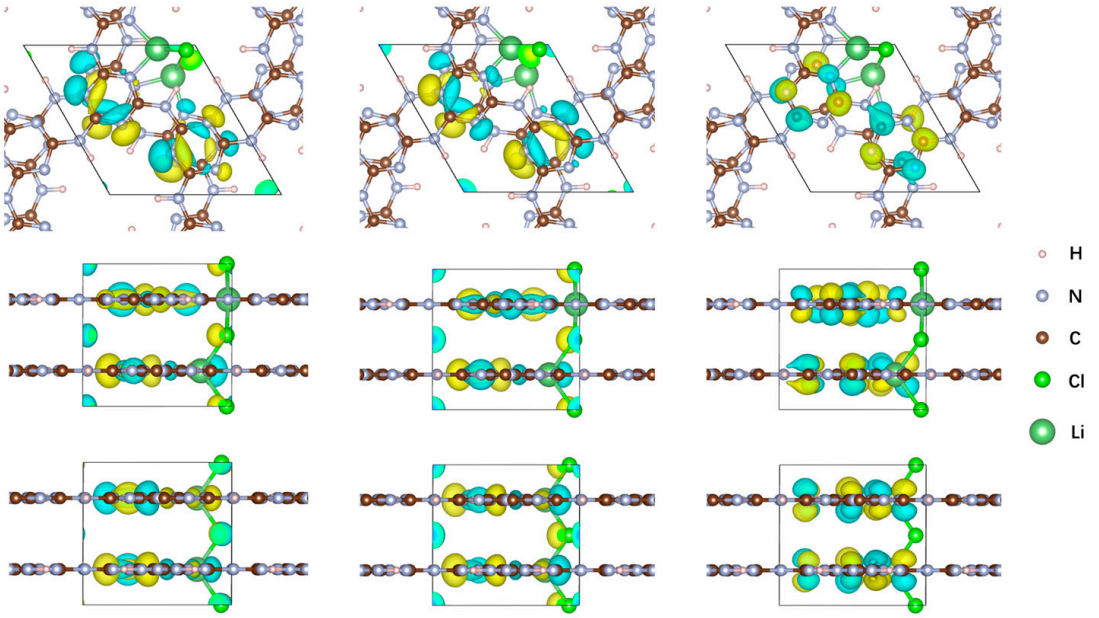

Figure S2. Representative band state at high symmetry point G, from left to right: band no. 81, band no.82, band no. 83.

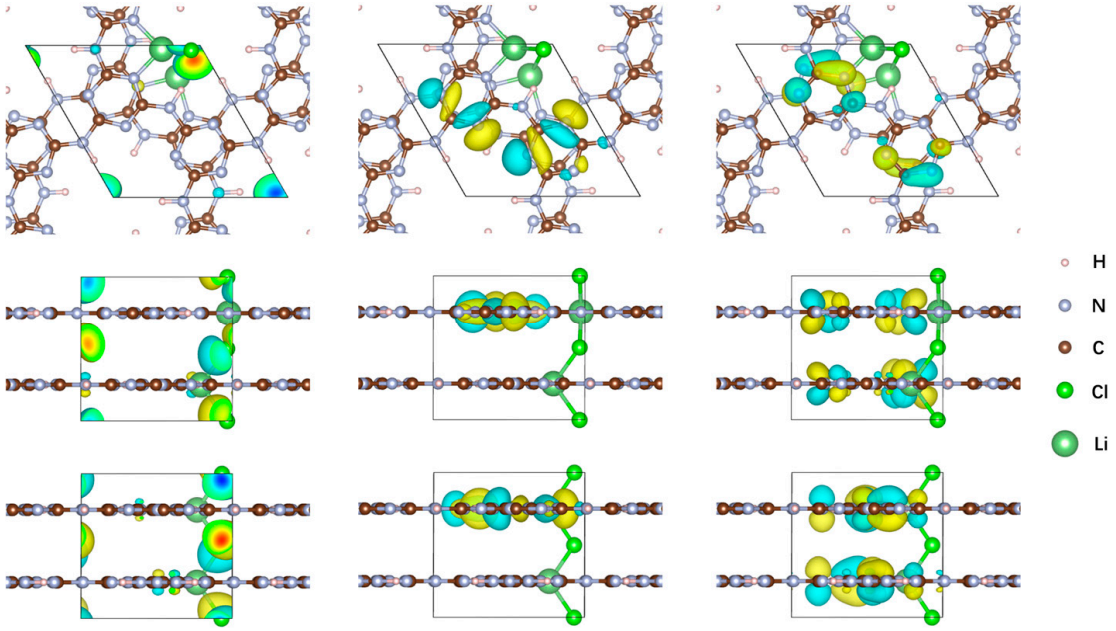

Figure S3. Representative band state at high symmetry point K, from left to right: band no. 81, band no.82, band no. 83.

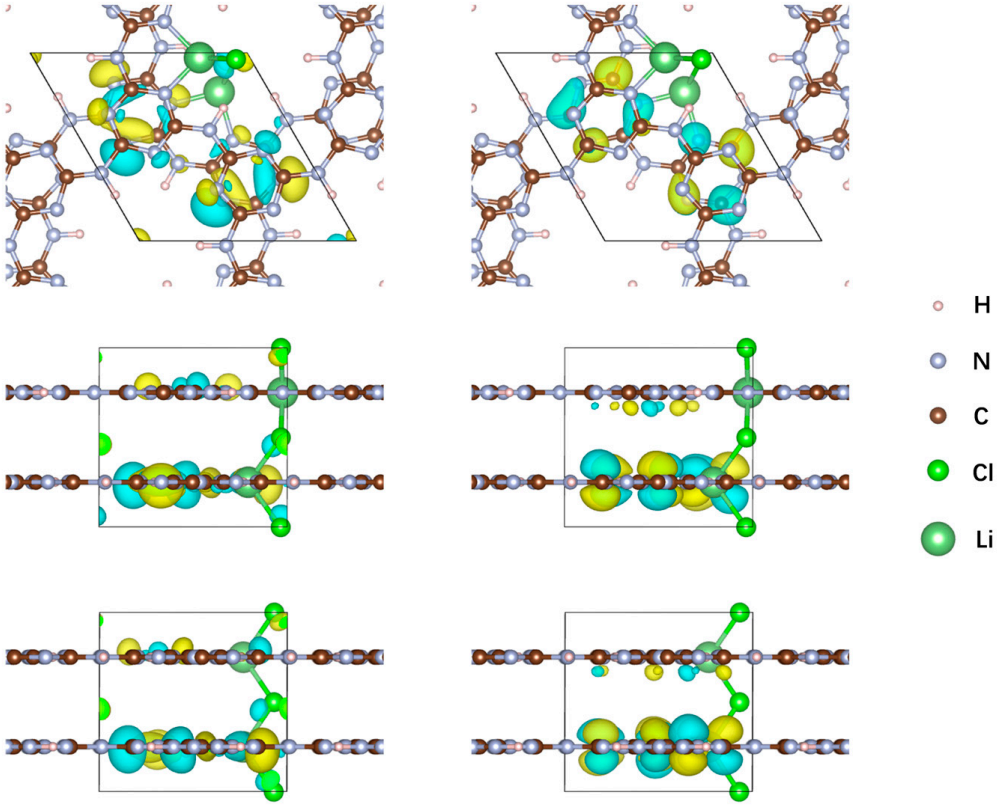

Figure S4. Representative band state at high symmetry point A, from left to right: band no. 82, band no.83

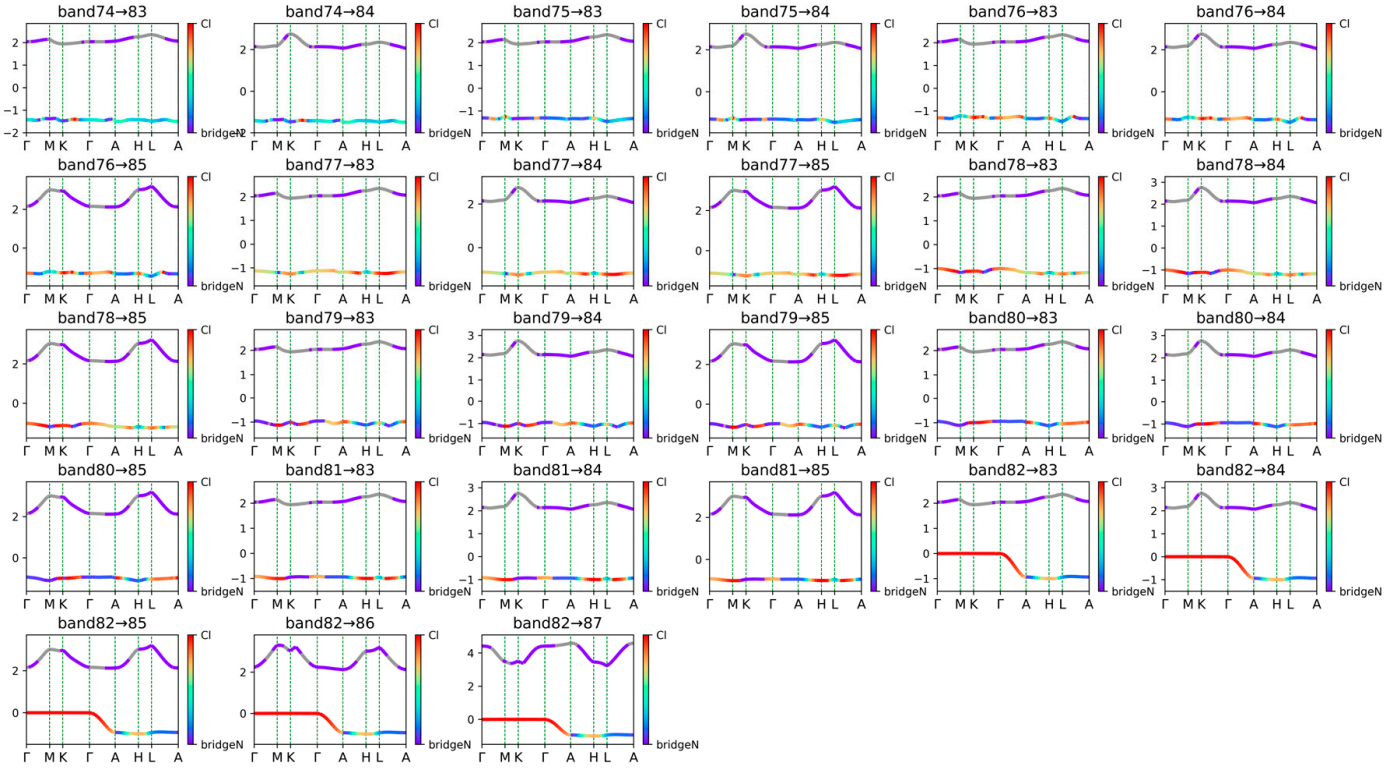

Figure S5. Contribution of p orbitals of bridgding N in each band, to confirm if the transition is concerned with the lone electron pairs.

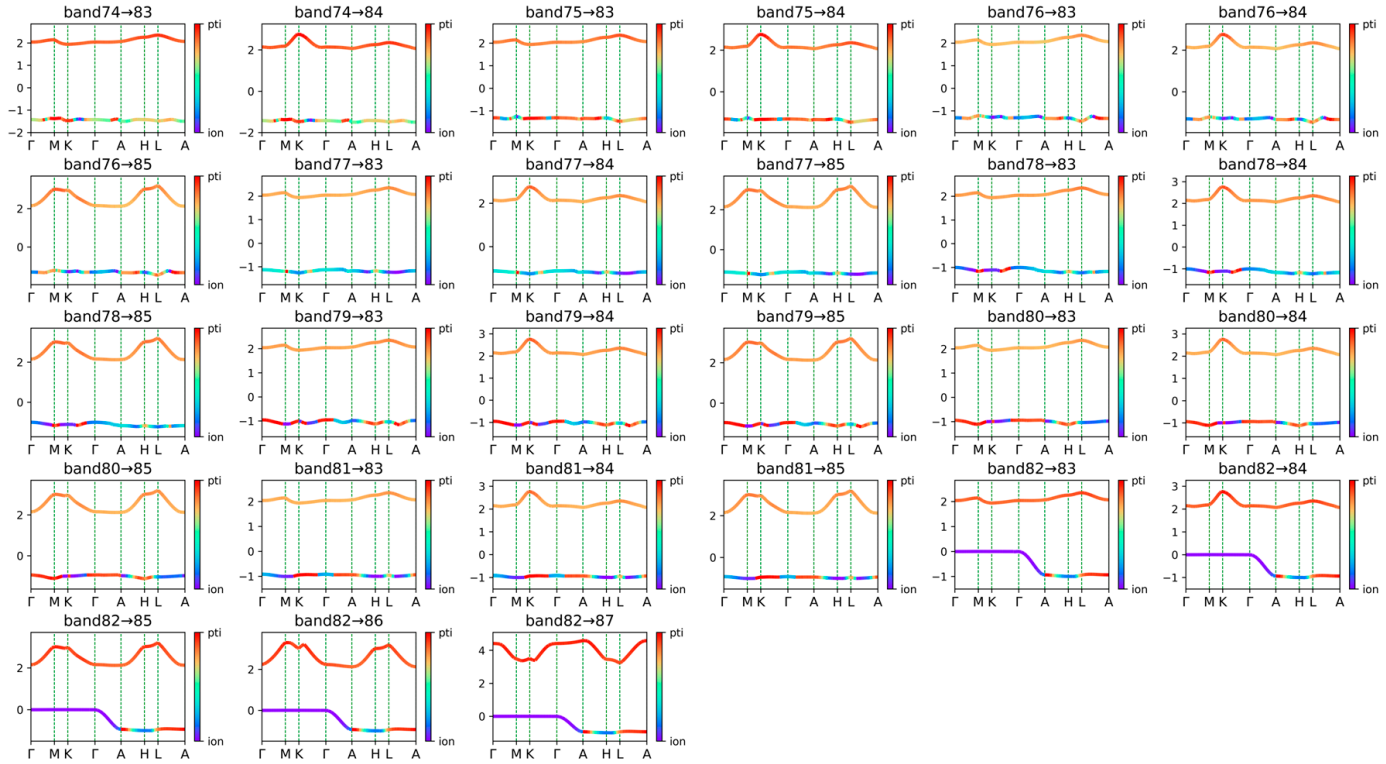

Figure S6. Relative compose of organic skeletons and ions in each band.

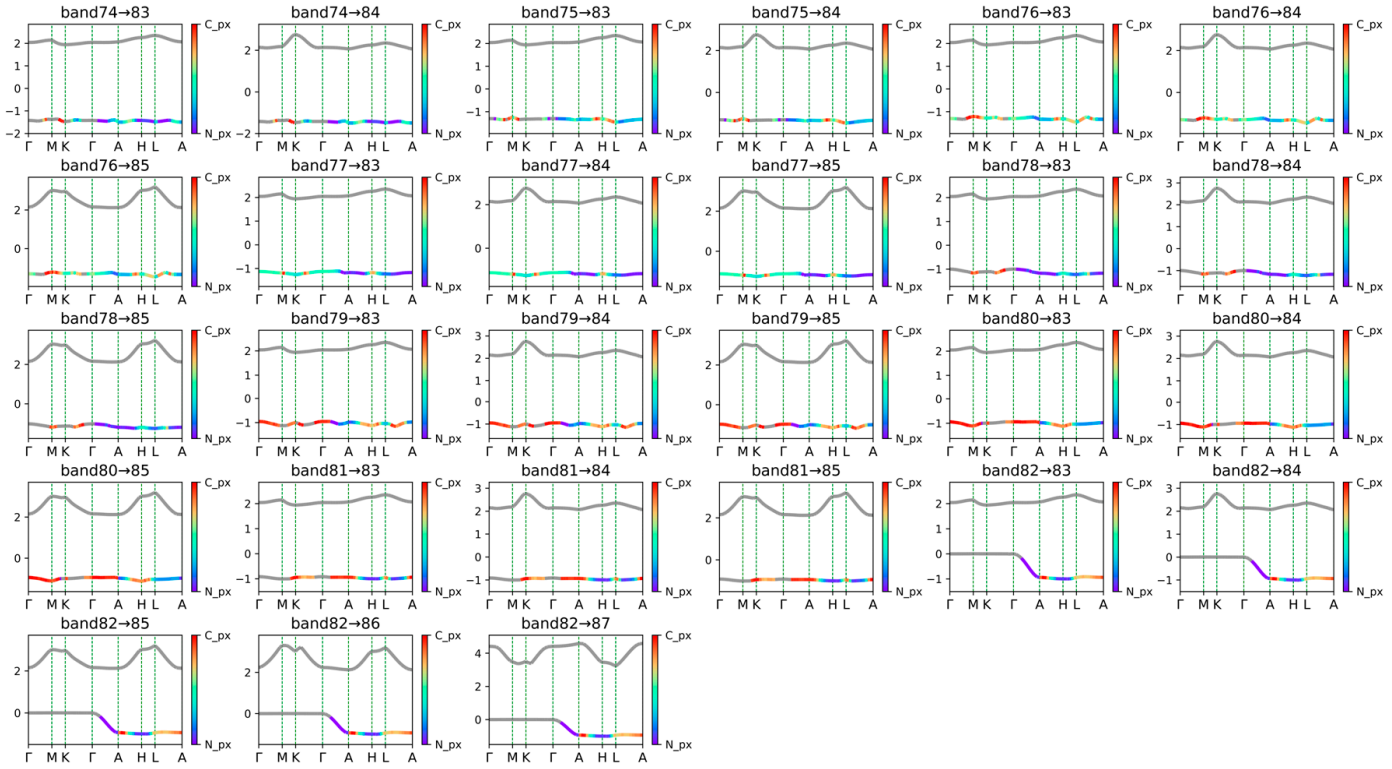

Figure S7. Contribution of p_x orbitals in each band, so that whether the excitation is involved with π-orbitals is ensured.

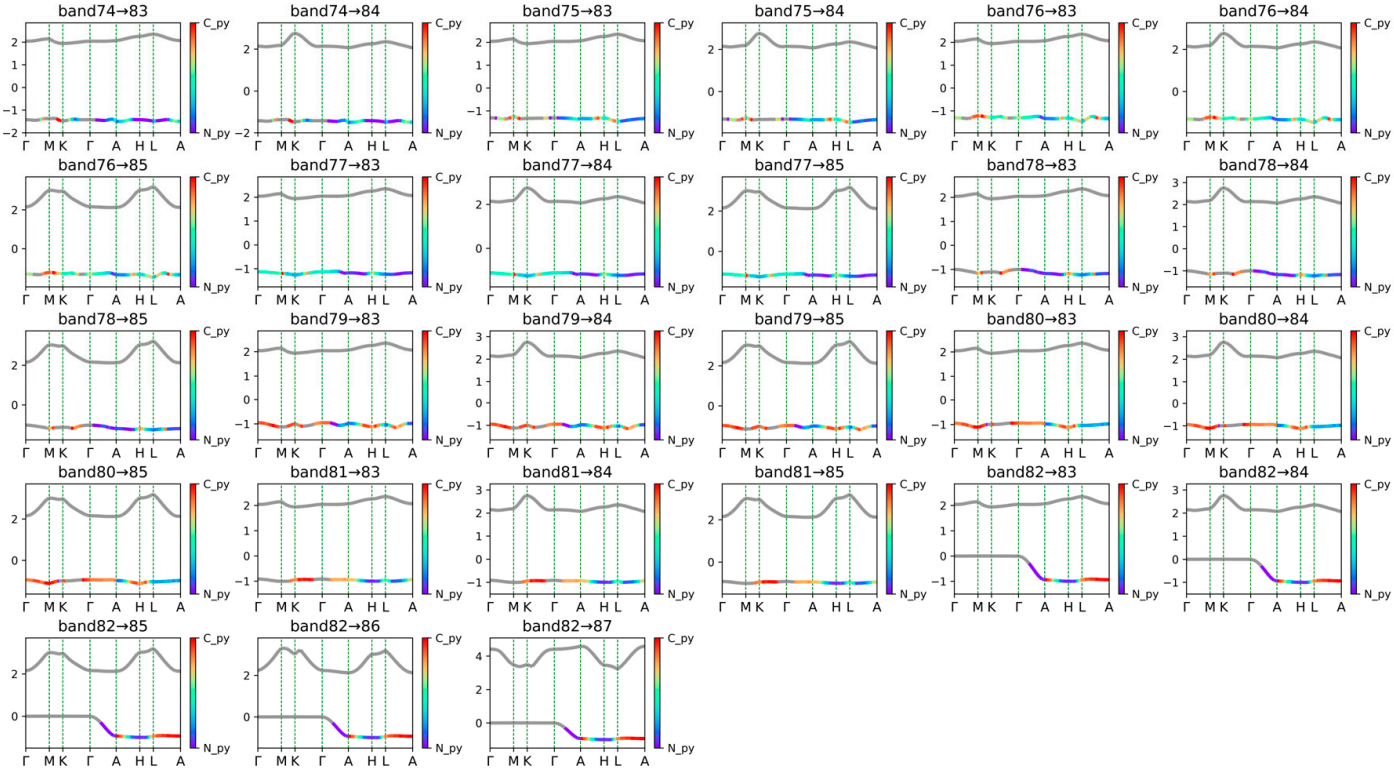

Figure S8. Contribution of p_y orbitals in each band, so that whether the excitation is involved with π-orbitals is ensured.

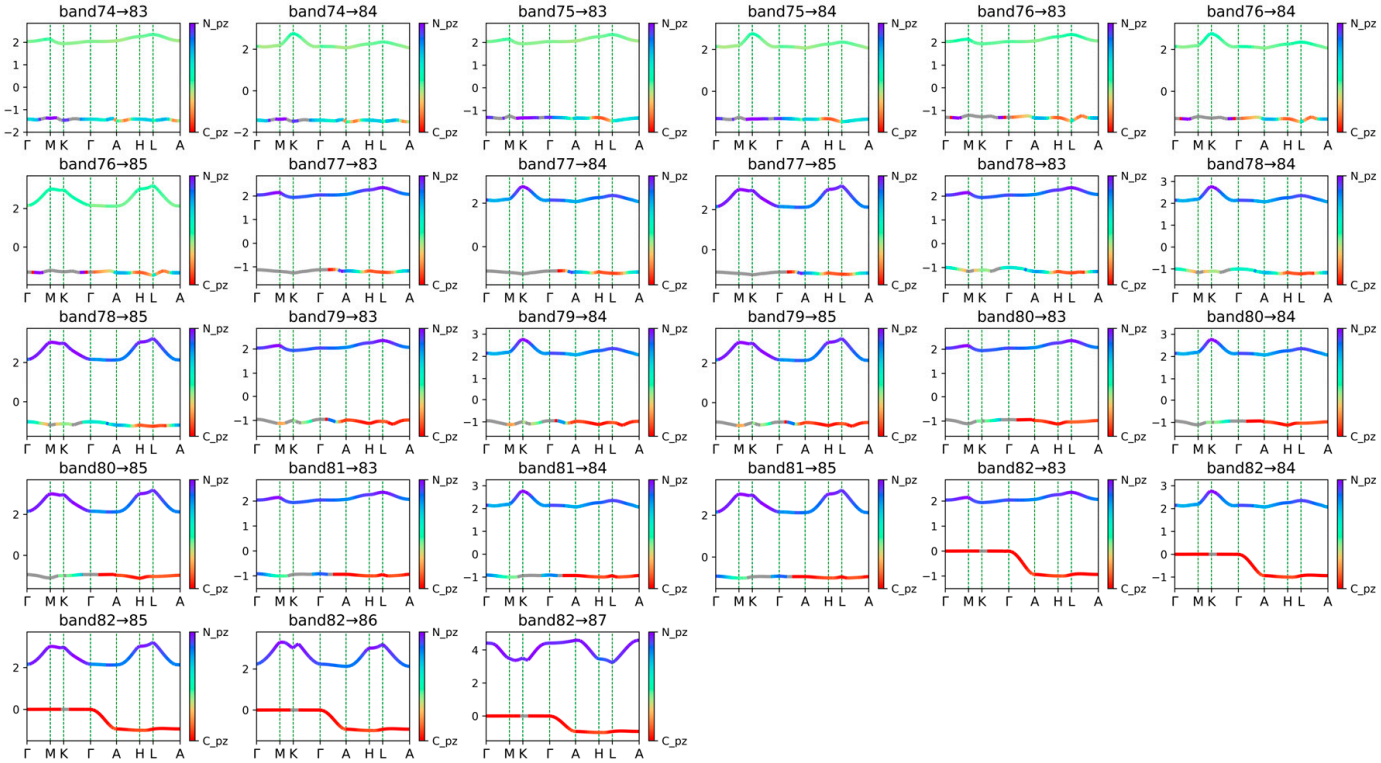

Figure S9. Contribution of p_z orbitals in each band, so that whether the excitation is involved with π-orbitals is ensured.

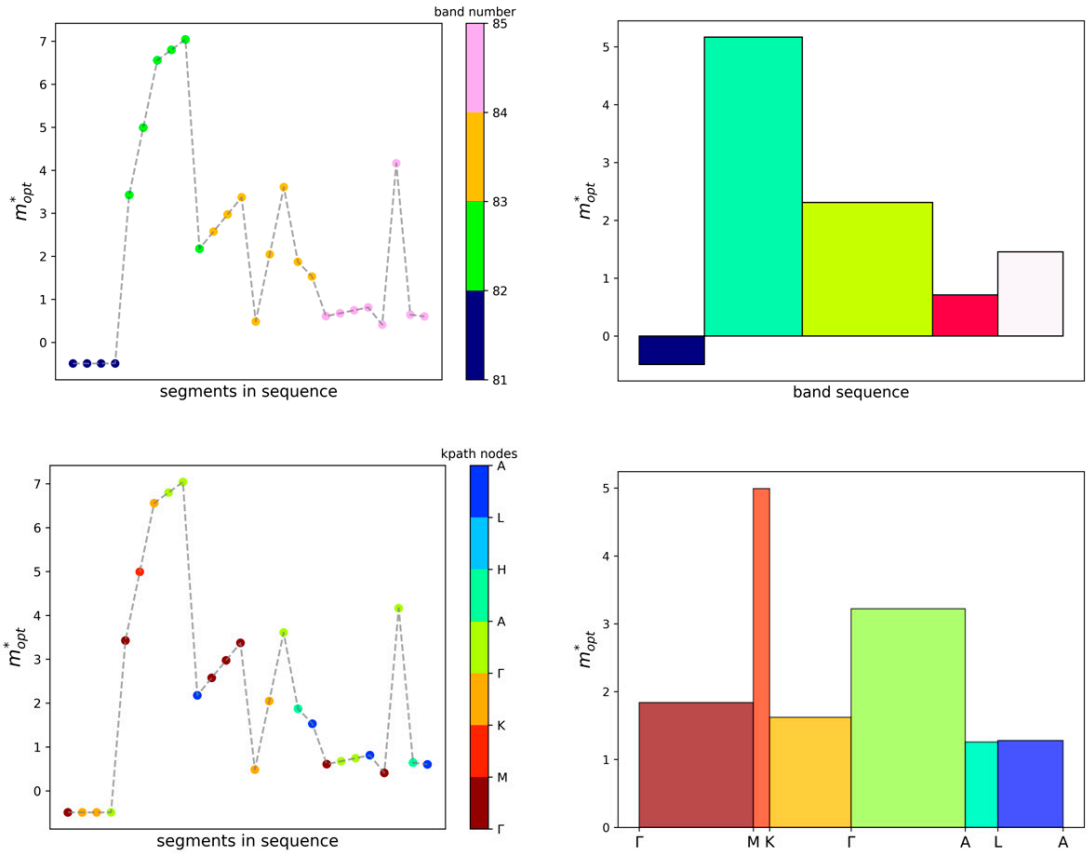

Figure S10. Optical effective mass of PTI/Li^+Cl^- calculated by Kane-dispersion, averaged by band number (upper) and k-points (lower), respectively. Segment in sequence is basically band segments separated by high symmetry K-points. As listed in Table S1, band sequence of horizontal axis included the band number from Band 82 is the ionic band of Li, has a relatively large effective mass.

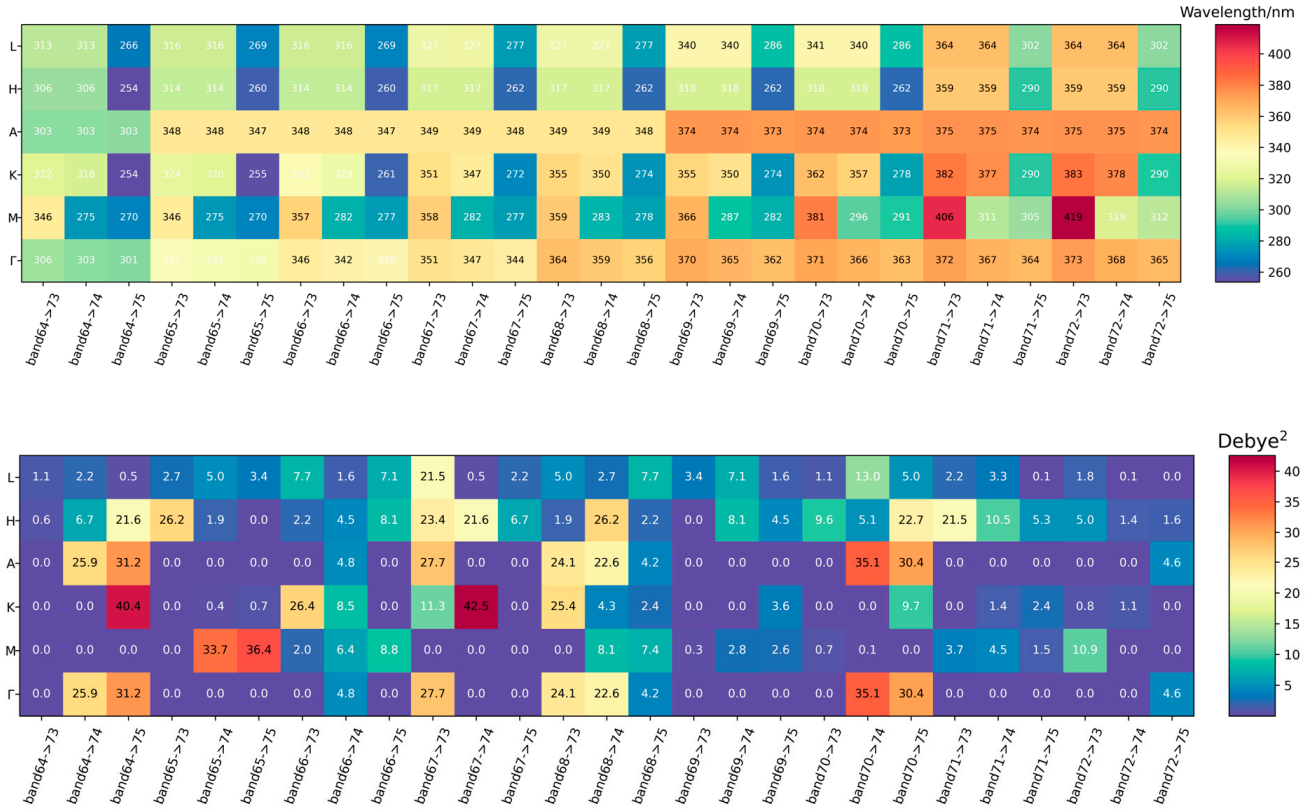

Figure S11. Screen matrix for binding energy and exciton radii

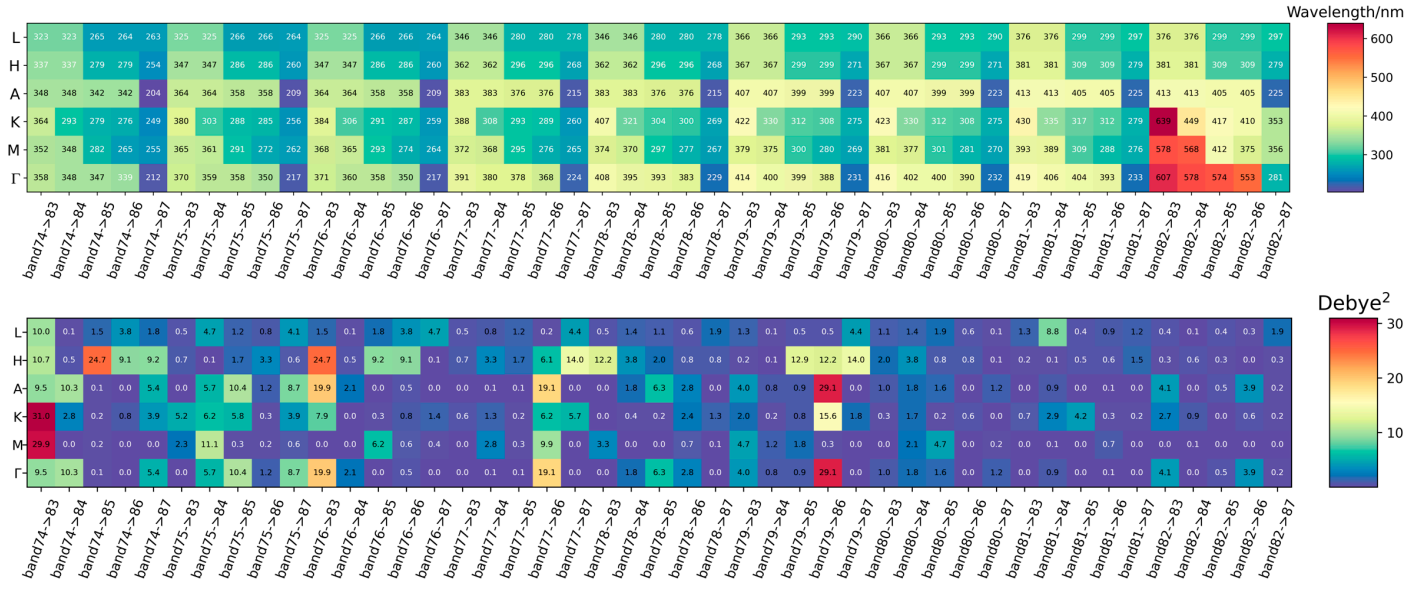

Figure S12. Screen matrix for binding energy and exciton radii, transition dipole moment matrix