Using the Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA) pseudopotential and plane wave basis method along with the frozen-phonon approach that starts from the ab initio evaluation of the total energy E_{tot} of the solid with frozen-in atomic displacements, it is found that a superposition of A_{2u} and the E_{2g}vibrations modes is the key factor in the superconducting mechanism in MgB_2 compound. Electron–Phonon coupling to these A_{2u} and E_{2g} phonon modes especially at the zone-boundary A point of the hexagonal Brilliouin zone leads to an interband hole charge transfer (and transfer back) between in-plane σ bond to the out-of-plane π bond along with an interatomic electron charge transfer (and transfer back) between the Magnesium s-states to the Boron out-of-plane p_z-state. The direction of the electronic current is opposite to that of hole current so that it reinforces the polarization associated with these currents and may generate a large dynamical charge at a given critical temperature T_c that drives the compound into the superconducting state