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Suplementary Materials

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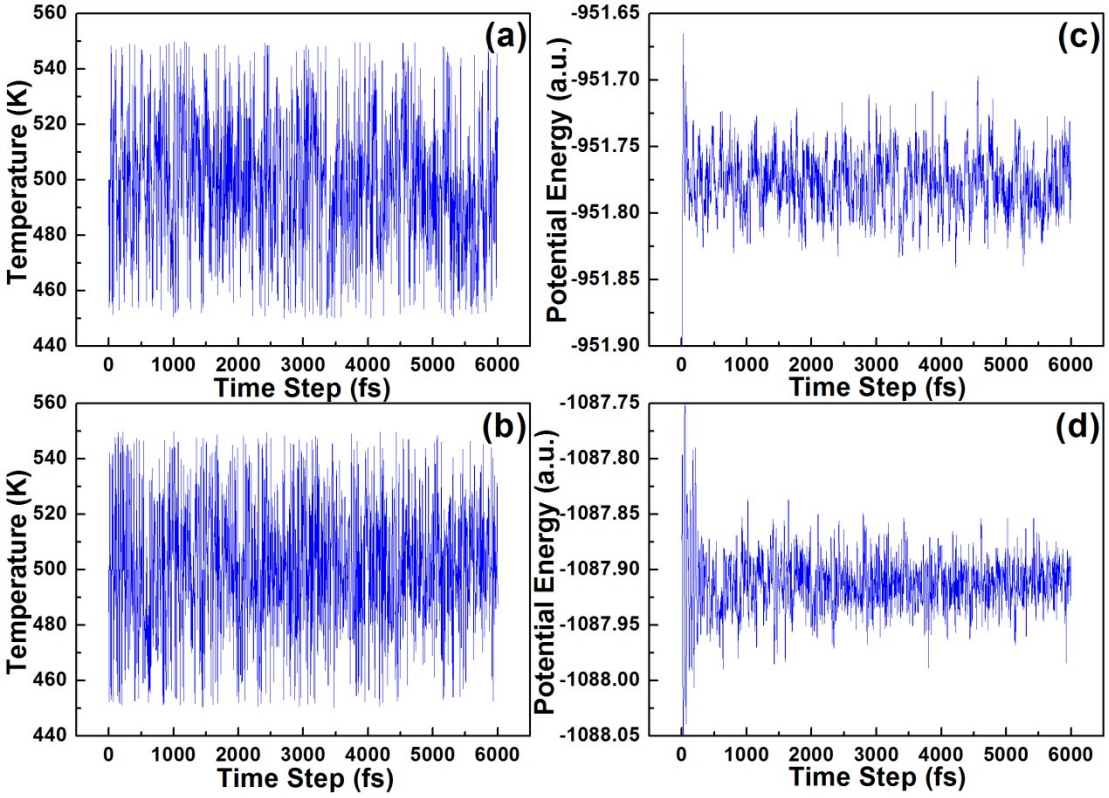

Fig. S1 (a) and (b) are the temperature of C_y and C_z in function of time steps, respectively. (c) and (d) are the total energy of C_y and C_z in function of time steps, respectively. All data were obtained by performing ab initio molecular dynamics simulations.

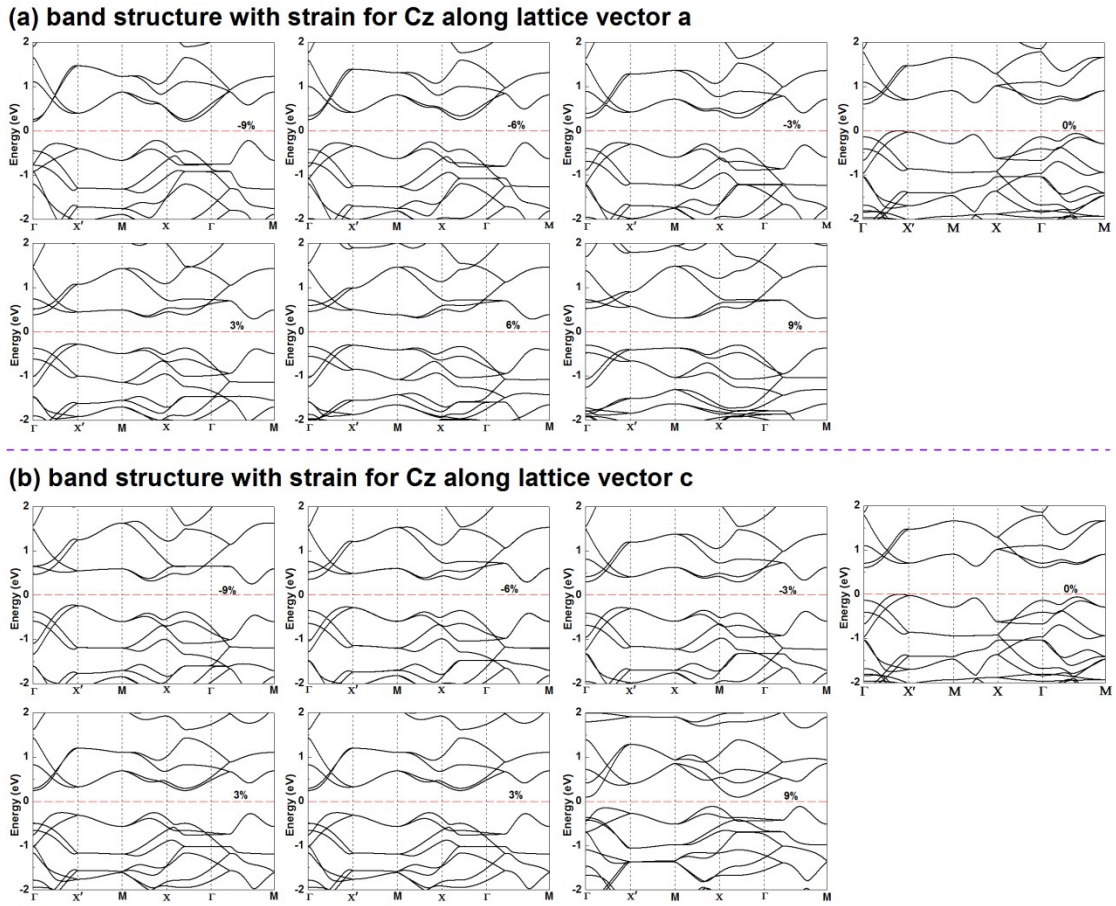

Fig. S2: (a) and (b) show the band gap as a function of strain for C_y and C_z.