Supplementary Material

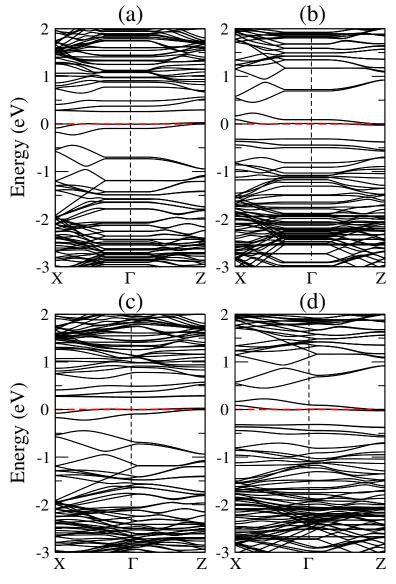


Figure 1: Eletronic band structure for the B_3N_6 and B_6N_3 defects. Panels (a) and (b) refer to the enlarged unit cell while (c) and (d) refer to the LYP functional.