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Table S1 Total energies for the spin states (M=1, 3 and 5) of the pristine and defective BC_3 sheets (including the vacancy of B (V_B) and C atoms (V_C)).

pri-BC_3	Total energy	V_B-BC_3	Total energy	V_C-BC_3	Total energy
M=1	-268.726 eV	M=1	-257.016 eV	M=1	-255.083 eV
M=3	-267.790 eV	M=3	-256.413 eV	M=3	-254.504 eV
M=5	-266.120 eV	M=5	-255.095 eV	M=5	-253.494 eV