Semiconducting Monolayer Materials as a Tunable Platform for Excitonic Solar Cells

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As stated in main text, the *GW* corrections for the three CBN monolayers $C_1(BN)_7$, $C_4(BN)_4$ and $C_7(BN)_1$ were taken from our previous work (ref. 15 of main text). Such corrections decrease approximately linearly for increasing C domain size, so that corrections at intermediate number of C atom rows can be derived by interpolation. Figure 1(a) below shows a linear interpolation of the *GW* corrections, yielding an error of ~ 0.1 eV – namely the same as the convergence error in our calculations – at all C domain sizes. In order to better fit the data, we employed a parabolic fit with very small curvature, also shown in Figure 1(a), though choosing the linear fit would only change the resulting efficiencies in Figure 2(b) of main text by less than 1%. The BSE corrections to the *GW* gap, expressed in terms of exciton binding energies, also scale linearly with C domain size, and were fitted with a straight line to obtain CBN optical gaps at intermediate C domain sizes [Figure 1(b)]. On the basis of these fits, an error of 0.1 eV (shown in both plots in Figure 1 below) is assumed on both the V_{oc} (deriving from the error on the *GW* correction) and on the optical gap (deriving from the error on the exciton binding energy). For simplicity, these two sources of error are assumed to be independent in our error analysis carried out in main text.

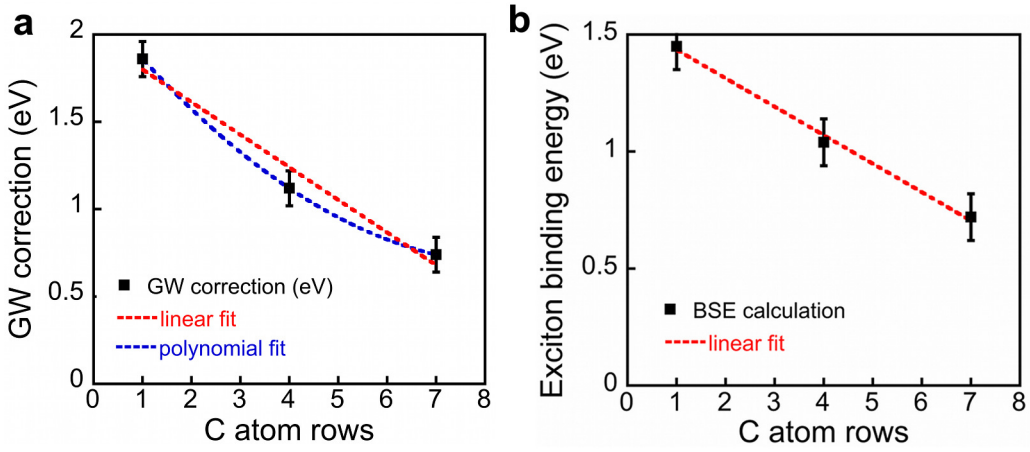

Figure 1: (a) Linear and parabolic fits used to determine the *GW* corrections for the CBN monolayers used in this work. (b) Linear fit for the exciton binding energies calculated within BSE. For both the *GW* and BSE corrections, the values are plotted as a function of the number of C atom rows x in the unit cell $C_x(BN)_{(8-x)}$, and error bars of 0.1 eV are shown.