1 ZPL calculations: PBE

$$\lambda = \frac{hc}{E} \tag{1}$$

where $h = 4.135667696 \times 10^{-15}$ eV.s and $c = 3 \times 10^{8}\ \frac{m}{s}$. Therefore $hc = 1241$ eV.nm.

Table 1: ZPL for PBE functional

Defect	Charge	Spin	Ground state (eV)	Excited state (eV)	ZPL (eV)	λ (nm)
V_B	-1	1	-1861.996779	–	–	–
N_B (up)	0	0	-1876.292874	-1874.517596	1.775278	699.045
N_B (down)	0	0	-1876.292874	-1874.517596	1.775278	699.045
N_B	+1	$1/2$	-1885.827992	-1884.158650	1.669342	743.407
$V_B - C_B$	0	1	-1870.327550	-1869.912551	0.414999	2990.369
(*) $V_B - C_B$	-1	$1/2$	-1861.844401	-1861.288752	0.555649	2233.434
$V_B - V_N$	0	1	-1859.307087	-1859.196933	0.110154	11266.046
(*) $V_B - V_N$	-1	$1/2$	-1850.949743	-1850.281175	0.668568	1856.206
$V_B - Si_B$	0	1	-1868.037273	-1867.633985	0.403288	3077.206
$V_B - Si_B$	-1	$1/2$	-1859.500205	–	–	–

2 ZPL calculations: HSE06

Table 2: ZPL for HSE06 functional

Defect	Charge	Spin	Ground state (eV)	Excited state (eV)	ZPL (eV)	λ (nm)
V_B	-1	1	-2174.505146	–	–	–
N_B (up)	0	0	-2190.499841	-2188.573660	1.926181	644.280
N_B (down)	0	0	-2190.499841	-2188.573660	1.926181	644.280
N_B	+1	$1/2$	-2200.668775	-2199.028439	1.640336	756.552
$V_B - C_B$	0	1	-2183.891363	-2182.958692	0.932671	1330.587
$V_B - C_B$	-1	$1/2$	-2175.171642	–	–	–
$V_B - V_N$	0	1	-2170.126715	-2169.300912	0.825803	1502.780
$V_B - V_N$	-1	$1/2$	–	–	–	
$V_B - Si_B$	0	1	-2181.164446	-2179.908609	1.255837	988.186
$V_B - Si_B$	-1	$1/2$	-2172.494346	–	–	–