



TABLE II. Calculated DFT, HSE06, and GW band gaps Δ_i and Δ_i^{HSE06} for $\text{C}_t\text{T}_i(\text{S,Se})_2$ ($\text{T}, \text{S,Se}$; N, CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH).

Material ($\text{C}_t\text{T}_i\text{X}_2$)	Band gap (eV)			Band gap assignment		
	DFT	HSE06	c-GW	DFT	HSE06	c-GW
$\text{C}_t\text{T}_i\text{S}_2$ (CH)	-0.77	0.06	-0.41	T	N	T
$\text{C}_t\text{T}_i\text{Se}_2$ (CH)	-1.0	-0.4	-0.85	T	T	T

calculated DFT. We compare c-GW and HSE06 band gaps Δ_i and Δ_i^{HSE06} for $\text{C}_t\text{T}_i(\text{S,Se})_2$ ($\text{T}, \text{S,Se}$; N, CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH). The band gap assignments are given in Table II. The band gap assignments are given in Table II.

For $\text{C}_t\text{T}_i(\text{S,Se})_2$ ($\text{T}, \text{S,Se}$; N, CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH), the band gap assignments are given in Table II. The band gap assignments are given in Table II. The band gap assignments are given in Table II.

Is HSE06 the answer? Recently, *Chen et al.*⁹ determined the band gap of $\text{C}_t\text{T}_i(\text{S,Se})_2$ ($\text{T}, \text{S,Se}$; N, CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH) using HSE06.¹⁰ We compare HSE06 and c-GW band gaps Δ_i and Δ_i^{HSE06} for $\text{C}_t\text{T}_i(\text{S,Se})_2$ ($\text{T}, \text{S,Se}$; N, CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH). The band gap assignments are given in Table II. The band gap assignments are given in Table II.

For $\text{C}_t\text{T}_i(\text{S,Se})_2$ ($\text{T}, \text{S,Se}$; N, CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH), the band gap assignments are given in Table II. The band gap assignments are given in Table II. The band gap assignments are given in Table II.

Conclusion. We compare HSE06 and c-GW band gaps Δ_i and Δ_i^{HSE06} for $\text{C}_t\text{T}_i(\text{S,Se})_2$ ($\text{T}, \text{S,Se}$; N, CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH). The band gap assignments are given in Table II. The band gap assignments are given in Table II.

We add the band gap assignments for $\text{C}_t\text{T}_i(\text{S,Se})_2$ ($\text{T}, \text{S,Se}$; N, CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH) and $\text{C}_t\text{T}_i(\text{S,Se})_2$ (CH) in Table II. The band gap assignments are given in Table II. The band gap assignments are given in Table II.

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