Supporting Information for

Characterization of large vacancy clusters in diamond from a generational algorithm using tight binding density functional theory

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\[ V_6 \]

\[ V_{10} \]

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Figure S1. Unrelaxed structures of selected vacancy clusters $V_n$ ($n=6, 10, 14, 19, 26, 30, 35, 39, 45, 50, 54$). Not that these structures turned out to be the most stable for the given $n$ after geometry relaxation.
Figure S2. Relaxed structures of selected vacancy clusters $V_n$ ($n=6, 14, 19, 26, 30, 39, 45, 50, 54$). These structures are the most stable for the given $n$ values. Larger blue atoms indicate those that are adjacent to the pore left by the vacancy cluster and undergo the largest rearrangement upon relaxation. As $n$ increases, regions of local graphitization become energetically favorable. For each $V_n$ different views are provided to aid the visualization.
$g(r)$ vs. $r / \text{Å}$

$V_6$

$V_{14}$
Figure S3. Calculated pair correlation function, $g(r)$ for $V_n$ in the $1.3 \, \text{Å} < r < 2.4 \, \text{Å}$ range. ($n=6, 14, 19, 26, 30, 39, 45, 50, 54$).
Figure S4. Calculated bond angle distribution function, $P$, for $V_n$ in the $90 < \Theta < 130$ range. No angles are observed outside the presented range. ($n=6, 14, 19, 26, 30, 39, 45, 50, 54$).