Supplementary Information

for

Dominant Luminescence is not Due to Quantum Confinement in Molecular-Sized Silicon Carbide Nanocrystals

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Stacking faults are two-dimensional defects in SiC crystal where the sequence of Si–C bilayers deviates from the perfect stacking sequences (along c-axis) of the crystal. Polytypes of SiC may be considered as regular pattern of "stacking faults" for long distances along the c-axis. The three common polytypes of SiC are shown in **figure S1 a-c**. While the mechanical properties of different polytypes are the same, their electronic properties vary considerably: the most known differences are the band gaps variation and band edge offsets. The indirect band gaps vary from 2.4 to 3.3 eV as the hexagonality increases from 0% (3C–SiC, cubic SiC) to 100% (2H–SiC)[1]. The conduction band offset between the cubic and hexagonal polytypes is large while the valence band offset is minute[3]. Whilst cubic silicon carbide (3C-SiC) exhibits only cubic sequences that might be described as a single straight line (see **figure S1a**), hexagonal 2H-SiC contains only hexagonal sequences that results in a zig-zag line. Other hexagonal phases such as 6H-SiC (see **figure S1c**) contain the combination of zig-zag and straight lines. In SiC stacking faults often occur that may result in polytype inclusions with the corresponding order of sequences too. The conduction band electrons can be confined in 3C-SiC regions in one dimension (3C region in 6H SiC or 6H inclusions in 3C SiC, for example, **figure S1d**). These bound electrons around the stacking

faults can move freely along the wells, and can be thought as two-dimensional electron gases in bulk material, but in the case of nanocrystals the other two dimensions are also finite because of the small crystal size.

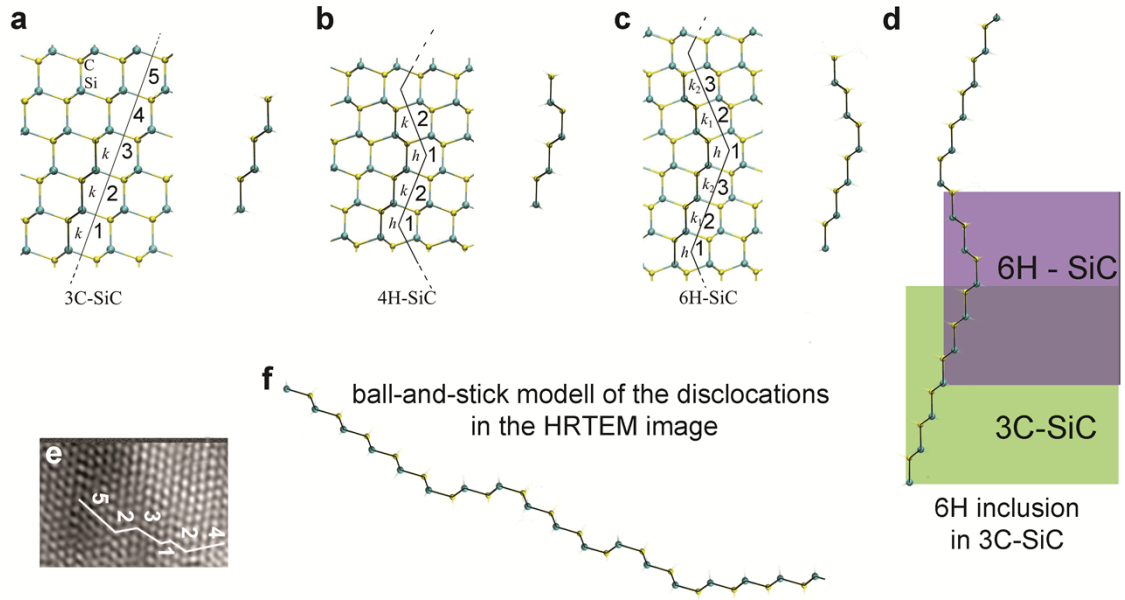

Figure S1: a-c: ball-and-stick representation of common SiC polytypes namely 3C-SiC, 4H-SiC, 6H-SiC. The values count the number of Si-C bilayers and reset it to one after a hexagonal layer has been passed. **d** represents 6H inclusion in 3C-SiC. **e** is the FFT combined HRTEM of 10 nm SiC nanocrystals with "irregular" stacking faults. Every dot in the image is a Si-C pair. Straight lines represent the cubic (3C) structure of the crystal while at every turn a hexagonal layer resides. The values represent the number of Si-C bilayers between two hexagonal layers. **f** is the ball-and-stick model of the SiC structure in TEM image. That shows a stacking fault region that might be considered as polytype inclusions together with stacking faults within polytype inclusions or simply irregular Si-C sequences. The measured lattice constants in HRTEM measurements support that mainly 3C and 6H polytypes occur in our SiC aggregates.

References:

(1) Patrick, L.; Hamilton, D. R.; Choyke, W. J. *Phys. Rev.* **1964**, *133*, A1163.

(2) Iwata, H. .; Lindefelt, U.; Öberg, S.; Briddon, P. . *Phys. B Condens. Matter* **2003**, *340-342*, 165–170.

(3) Davydov, S. Y. *Semiconductors* **2007**, *41*, 696–698.