Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for PCCP

Surface-state dependent optical properties of OH-, F-, and H-terminated 4H-SiC quantum dots

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(Dated: 7th July, 2016)

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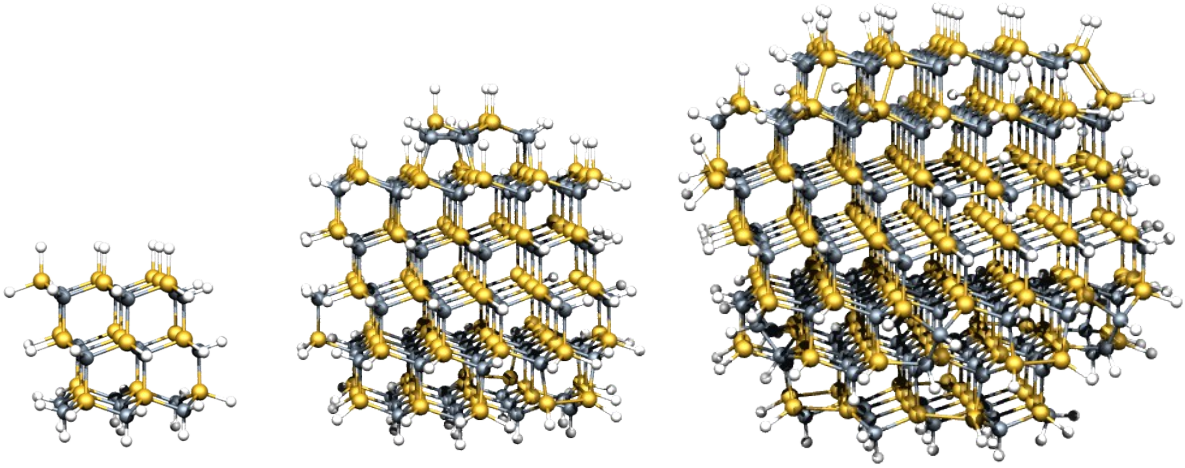
Fig. 1 Optimized structures of Si-centered (a) 10 Å, (b) 16 Å and (c) 20 Å diameter H-terminated QDs.

Table. 1 Table listing of SiC-QD cluster composition as a function of QD diameter.



(a) (b) (c)

Fig. 1 Optimized structures of Si-centered (a) 10 Å, (b) 16 Å and (c) 20 Å diameter H-terminated QDs.

Diameter (Å)	$N_{Si}(Si), N_C(C)$	$N_{Si}(C), N_C(Si)$	$N_{Surface}$	$N_{recon.}(Si)$	$N_{recon.}(C)$
10	19	20	40	40	40
11	29	29	56	44	44
12	51	41	82	70	70
13	57	62	94	76	76
14	69	74	100	88	88
15	81	83	112	100	100
16	99	96	126	114	114
17	132	118	160	130	136
18	147	151	172	130	142
19	159	175	190	160	148
20	207	199	208	166	172

Table 1. SiC-QD cluster composition as a function of QD diameter. The numbers of Si and C atoms, $N_{\mathrm{Si}}(X)$ and $N_{\mathrm{C}}(X)$, listed in the table refer to the X-centered SiC-QD. N_{Surface} lists the number of surface sites on the unreconstructed clusters, which is independent of whether the QD is Si or C centered. For reconstructed clusters the number of surface sites is different for Si and C centered cases, with the total number of surface sites on reconstructed X-centered SiC-QDs being $N_{\mathrm{recon.}}(X)$.