

Supporting Information: Silicon Clathrate Quantum Dots and the Allotropic Dependence of Quantum Confinement

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Table 1: Confinement constants and reduced effective masses for diamond silicon, clathrate types I-VIII and type H.

Structure	dSi	I	II	III	IV
$A^{(EMA)}, \text{Ha-a}_0^2$	68.97	30.66	44.44	36.24	36.47
m^*	0.13	0.29	0.24	0.29	0.29
Structure	V	VI	VII	VIII	Type H
$A^{(EMA)}, \text{Ha-a}_0^2$	40.28	21.45	54.56	37.07	42.29
m^*	0.35	0.57	0.15	0.24	0.20

Table 2: Calculated values of effective mass, m^* , for various well known structures.

Valence Band	m^*	m^*	% Error	Error (abs)
dSi	0.36	0.26	27.50	0.1
dGe	0.21	0.22	5.71	0.01
dC	0.47	0.55	16.93	0.08
GaAs	0.34	0.28	17.94	0.06
Conduction Band	m^*	m^*	% Error	Error (abs)
dSi	0.26	0.25	4.23	0.01
dC	0.36	0.40	12.29	0.04
GaAs	0.07	0.01	84.18	0.05