Preferential positioning of dopants and co-dopants in embedded and freestanding Si nanocrystals

SUPPLEMENTARY INFORMATIONS

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S1 – TOTAL ENERGIES

We report in the next table the total energies for the single-doped Si_{35}/SiO_2, expressed in eV (see Figure 2 in main article):

position	B	P	N	Al
dot	-189267.6576	-189360.2563	-189448.8667	-189237.5461
interface1	-189268.0927	-189359.7617	-189447.4560	-189237.8686
interface2	-189268.6112	-189358.3333	-189444.3560	-189238.0789
silica	-189267.4836	-189356.4857	-189441.0240	-189236.4543

We report in the next table the total energies for the co-doped freestanding Si_{87} NC, expressed in eV (see Figure 5 in main article):

index	energy	positions
5	-43735.825263	P center, B surface
4	-43736.067600	P center+1, B surface
3	-43736.396667	P center+2, B surface
2	-43736.690502	P center+3, B surface
1	-43737.193174	P center+4 (=surface-1), B surface
1c	-43736.906137	P center, B center+1
1i	-43735.746888	P surface, B surface-1
esa1	-44004.032836	six B-P pairs, two for each axis
esa1i	-44004.005199	six B-P pairs, two for each axis, one B-P pair switched

S2 - BOND LENGTHS

We report in the table below the length of the bonds, in Angstrom units, formed by the dopant with its neighbours, for different dopant site in the Si_{35} NC embedded in SiO_2 (see Figure 3 in main article):

core	**Si**	**Si**	**Si**	**Si**
N	2.01	2.11	2.04	2.20
P	2.41	2.48	2.43	2.48
Al	2.51	2.54	2.52	2.54
B	2.13	2.17	2.14	2.17
interface1	**Si**	**Si**	**Si**	**O**
N	1.82	1.81	3.46	1.46
P	2.41	2.39	2.39	1.69
Al	2.60	2.56	2.48	1.75
B	2.21	2.19	2.21	1.41
interface2	**Si**	**Si**	**O**	**O**
N	2.02	2.81	1.45	1.43
P	2.40	2.43	1.64	1.63
Al	2.56	2.58	1.74	1.73
B	2.11	3.31	1.36	1.37
silica	**O**	**O**	**O**	**O**
N	1.32	1.32	1.32	2.21
P	1.55	1.55	1.56	1.55
Al	1.73	1.73	1.75	1.73
B	1.44	1.45	1.47	1.47

S3 - DIPOLE MOMENTS

We report in the next table the calculated dipole moments for the undoped -H terminated NCs (see inset of Fig. 5 in the main article):

System	**d(nm)**	**dipole-moment(Debye)**
Si35-H36	1.06	0.117296
Si32-H56	1.12	0.18038
Si47-H60	1.21	0.338969
Si61-H66	1.31	0.00624924
Si87-H76	1.36	0.111831
Si71-H108	1.49	0.736794
Si109-H108	1.61	0.26173
Si147-H100	1.84	0.000804569
Si293-H172	2.15	0.0176253

We report in the next table the calculated dipole moments for the undoped -OH terminated NCs (see inset of Fig. 5 in the main article):

System	**d(nm)**	**dipole-moment(Debye)**
Si35-OH36	1.06	5.5
Si32-OH56	1.12	10.6
Si47-OH60	1.21	8.6
Si61-OH66	1.31	10.9
Si87-OH76	1.36	24.21
Si71-OH108	1.49	14.6
Si109-OH108	1.61	11.8
Si147-OH100	1.84	9.7
Si293-OH172	2.15	19.15

We report in the next table the calculated dipole moment, along the three directions and in module, for the undoped and co-doped Si_{87} freestanding NC(Debye units):

System	**dipole-X**	**dipole-Y**	**dipole-Z**	**module**
Si87_undoped	-3.321725	-15.878337	-17.971011	24.2098
Si87_codoped5	-10.42913	-15.076334	-17.548470	25.3774
Si87_codoped4	-9.128717	-12.982849	-15.305178	22.0485
Si87_codoped3	-7.421929	-14.575283	-14.042031	21.557
Si87_codoped2	-6.246769	-16.367848	-15.360312	23.2995
Si87_codoped1	-4.628061	-14.760621	-17.264075	23.1807
Si87_codoped1c	-3.313223	-16.937105	-19.162497	25.7885
Si87_codoped1i	-2.374841	-16.889131	-19.332235	25.7802
Si87_esa-codoped1	-5.939475	-13.268935	-17.350520	22.6359
Si87_esa-codoped1i	-10.126921	-15.405303	-12.676336	22.3734