– Electronic Supplementary Information –

Energetics and carrier transport in doped Si/SiO_2 quantum dots

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	$\mathbf{Si_{32}}$	$\mathbf{Si_{35}}$	$\mathbf{Si_{47}}$
E_g	2.74	1.82	2.01
EB	3.82	3.46	3.40
HB	4.41	4.76	4.82

TABLE S1: Undoped structures: HOMO-LUMO gap E_g, electron- and hole- barrier (EB, HB) – corrected values (see Method). All values are expressed in eV.

$\mathbf{Si_{32}}$	B-dot	B-int-1	B-int-2	**B-int-3**	B-silica
E_g	0.64	0.78	—	**0.70**	2.66
EB	3.91	3.68	—	**3.42**	3.96
HB	4.31	4.54	—	**4.80**	4.26
Δ_{HOMO}	0.96	1.12	—	**1.42**	-0.10
Δ_{LUMO}	-1.16	-0.86	—	**-0.65**	-0.20
ΔE_F	-0.10	0.13	—	**0.39**	-0.15

$\mathbf{Si_{35}}$	B-dot	B-int-1	**B-int-2**	B-int-3	B-silica
E_g	1.96	0.13	**0.50**	—	1.78
EB	3.49	4.24	**3.46**	—	3.78
HB	4.74	3.99	**4.76**	—	4.45
Δ_{HOMO}	0.02	0.19	**0.78**	—	-0.17
Δ_{LUMO}	0.16	-1.50	**-0.54**	—	-0.22
ΔE_F	-0.02	-0.77	**0.00**	—	-0.31

$\mathbf{Si_{47}}$	B-dot	B-int-1	B-int-2	**B-int-3**	B-silica
E_g	2.03	0.20	0.48	**0.58**	1.96
EB	3.38	4.18	3.58	**3.38**	3.57
HB	4.85	4.04	4.64	**4.84**	4.65
Δ_{HOMO}	0.04	0.15	0.61	**0.76**	-0.12
Δ_{LUMO}	0.06	-1.66	-0.92	**-0.67**	-0.17
ΔE_F	0.02	-0.78	-0.18	**0.02**	-0.17

$\mathbf{Si_{32}}$	**P-dot**	P-int-1	P-int-2	P-int-3	P-silica
E_g	**0.60**	0.29	—	0.25	0.10
EB	**3.27**	2.76	—	2.73	2.38
HB	**4.95**	5.46	—	5.49	5.84
Δ_{HOMO}	**1.63**	2.28	—	2.34	2.76
Δ_{LUMO}	**-0.54**	-0.19	—	-0.17	-0.10
ΔE_F	**0.54**	1.05	—	1.08	1.43

$\mathbf{Si_{35}}$	**P-dot**	P-int-1	P-int-2	P-int-3	P-silica
E_g	**0.00**	0.00	0.34	—	0.00
EB	**3.10**	2.81	3.09	—	2.46
HB	**5.12**	5.41	5.13	—	5.77
Δ_{HOMO}	**1.39**	1.68	1.23	—	2.03
Δ_{LUMO}	**-0.43**	-0.14	-0.24	—	0.22
ΔE_F	**0.36**	0.65	0.37	—	1.01

$\mathbf{Si_{47}}$	**P-dot**	P-int-1	P-int-2	P-int-3	P-silica
E_g	**0.12**	0.00	0.35	0.56	0.00
EB	**3.07**	2.69	3.04	3.41	3.63
HB	**5.15**	5.54	5.18	4.82	4.59
Δ_{HOMO}	**1.30**	1.74	1.21	0.75	0.79
Δ_{LUMO}	**-0.59**	-0.26	-0.44	-0.70	-1.21
ΔE_F	**0.33**	0.71	0.36	-0.01	-0.24

TABLE S2: Doped structures: HOMO-LUMO gap E_g; electron- and hole- barrier (EB, HB) – corrected values (see Method); shift of HOMO, LUMO, and E_F levels with respect to the undoped counterpart (Δ_{HOMO}, Δ_{LUMO}, and ΔE_F, respectively). All values are expressed in eV, with bold text highlighting the most stable configuration.

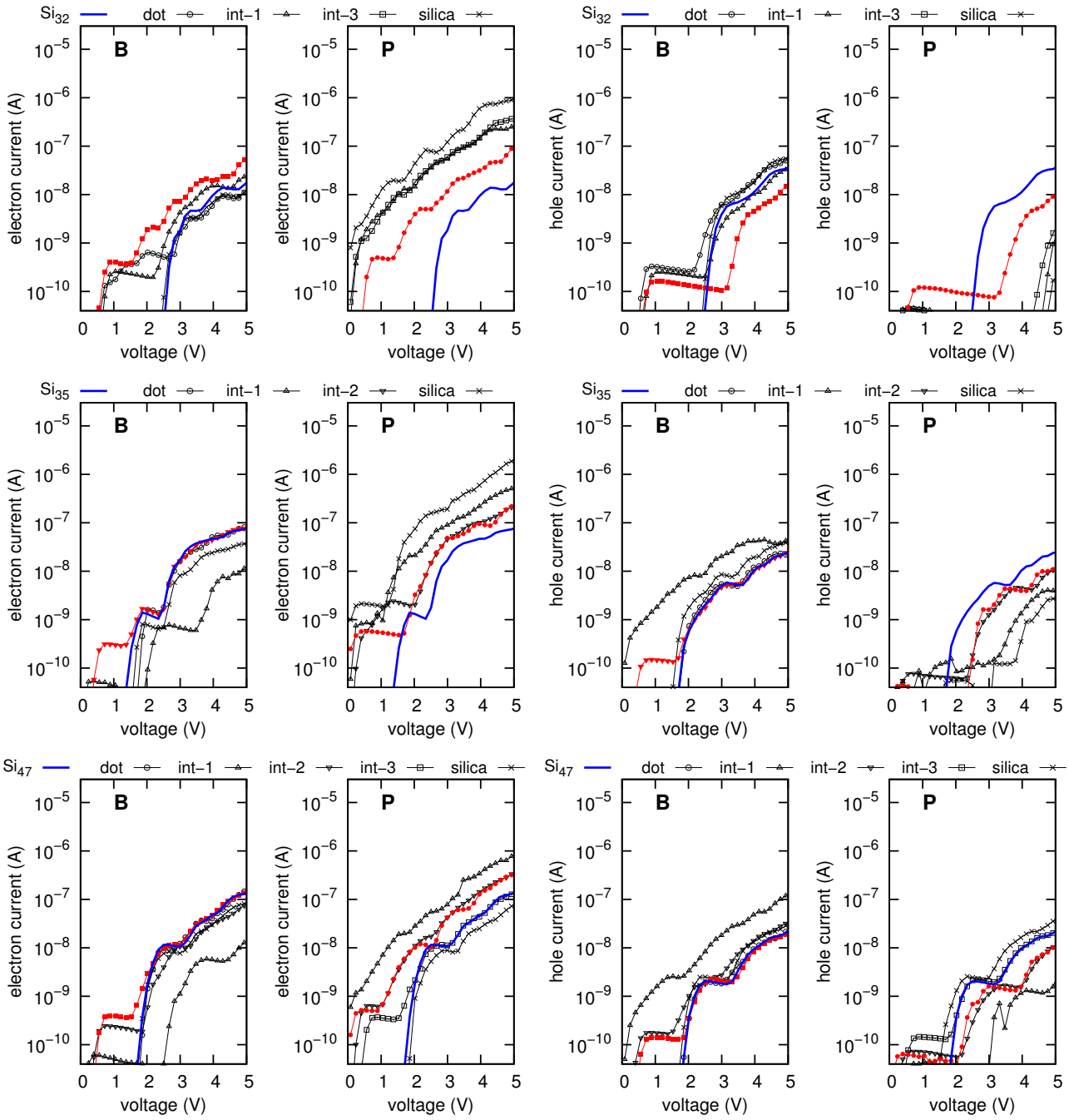

FIGURE S1: Separate electron and hole currents as a function of the applied voltage, for the considered doped configurations (symbols) along with the undoped case (blue solid curve), for Si_{32} (top), Si_{35} (center), and Si_{47} (bottom) QDs. Filled symbols (in red) highlight the most stable doped configuration.