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Supplementary Information

Clarifying effects of nanoscale porosity of silicon on the band gap and alignment: a combined molecular dynamics – density functional tight binding computational study

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Table S1: Computed band gap (E_g), the valence band maximum (VBM) and conduction band minimum (CBM), of the spherical pore models, along with its corresponding four initial box sizes (S(mall), M(edium), L(arge), XL (extra large)), number of atoms, and pore parameters: diameter (d), shortest (l) and largest (L) inter-pore distance.

Model label	Box Size	Number of Atom			d	L	l	Porosity	VBM	CBM	E_g
	[nm]	Si	H	Total	[nm]	[nm]	[nm]	[%]	[eV]	[eV]	[eV]
S1	2.17	425	204	629	1.47	2.25	0.86	16.2	-5.16	-3.62	1.54
S2		465	188	653	1.20	2.72	0.98	8.8	-5.10	-3.77	1.33
S3		495	164	659	0.92	3.02	1.52	4.0	-5.09	-3.88	1.21
M1	3.26	1263	540	1803	2.56	3.01	0.72	25.4	-5.15	-3.74	1.41
M2		1537	436	1973	2.02	3.64	1.26	12.5	-5.07	-3.90	1.17
M3		1681	348	2029	1.20	4.58	2.07	2.6	-5.07	-3.97	1.10
L1	4.34	2997	948	3945	3.37	4.12	0.98	24.4	-5.08	-3.86	1.22
L2		3631	764	4395	2.56	4.89	1.81	10.7	-5.05	-3.94	1.11
L3		3949	612	4561	1.74	6.06	2.61	3.4	-5.06	-3.99	1.07
XL1	4.89	4264	1200	5464	3.87	4.79	0.98	26.0	-5.06	-3.89	1.17
XL2		5126	1000	6126	2.74	5.96	2.07	9.2	-5.05	-3.95	1.10
XL3		5636	792	6428	2.03	7.15	2.88	3.8	-5.06	-4.00	1.06
c-Si		144	8	152	0	Bulk	Bulk	0	-5.03	-3.96	1.07

Table S2. Computed band gap (E_g) of the internal cube models, their valence band maximum (VBM) and conduction band minimum (CBM), along with its corresponding four initial box sizes (S, M, L, XL), number of atoms, and pore parameters.

Model Name	Box Size	Number of Atom			*d*	*L*	*l*	Porosity	VBM	CBM	E_g
	[nm]	Si	H	Total	[nm]	[nm]	[nm]	[%]	[eV]	[eV]	[eV]
S1	2.17	341	308	649	2.32	1.49	0.74	30.4	-5.32	-3.44	1.88
S2		417	252	669	1.99	1.77	1.00	16.0	-5.21	-3.63	1.58
S3		495	164	659	0.90	3.05	1.54	2.6	-5.09	-3.88	1.21
M1	3.26	863	828	1691	4.18	1.49	0.74	47.4	-5.33	-3.44	1.89
M2		1107	734	1831	3.87	1.77	1.00	33.8	-5.23	-3.58	1.65
M3		1449	540	1989	2.65	3.05	1.54	14.7	-5.12	-3.83	1.29
M4		1683	364	2047	1.39	4.27	2.36	2.4	-5.07	-3.98	1.09
L1	4.34	1625	1604	3229	6.07	1.49	0.74	58.3	-5.34	-3.44	1.90
L2		2133	1452	3585	5.75	1.77	1.00	45.8	-5.20	-3.58	1.62
L3		2931	1172	4103	4.52	3.05	1.54	27.1	-5.08	-3.79	1.29
L4		3669	852	4521	3.77	4.27	2.36	10.4	-5.06	-3.94	1.12
L5		4001	636	4637	2.01	5.52	3.15	2.1	-5.07	-3.99	1.08
L6		4091	524	4615	0.48	7.09	3.97	0.1	-5.07	-4.01	1.06
XL1	4.89	2096	2088	4184	7.01	1.49	0.74	62.6	-5.33	-3.45	1.88
XL2		2772	1912	4684	6.69	1.77	1.00	50.4	-5.19	-3.58	1.61
XL3		3870	1584	5454	5.46	3.05	1.54	32.2	-5.07	-3.78	1.29
XL4		4968	1192	6160	4.21	4.27	2.36	14.4	-5.05	-3.93	1.12
XL5		5552	904	6456	2.95	5.52	3.15	4.5	-5.06	-3.98	1.08
XL6		5786	720	6506	1.39	7.09	3.97	0.8	-5.07	-4.02	1.05
c-Si	-	144	8	152	0	Bulk	Bulk	0	-5.03	-3.96	1.07

Table S3. Computed band gap (E_g) of the pillar models, calculated by its valence band maximum (VBM) and conduction band minimum (CBM) along with its corresponding number of atoms, and pore features. The band gaps of the pillar and base part are calculated separately to investigate the effect of the local band gap. Four key features are varied to investigate the effect of each part: pillar diameter, pillar height, base layer, and interpillar distance with different pillar diameters. The varied features in each set are highlighted in bold.

Model Name		Number of Atom			Height	Base	Pillar Diameter	Distance		Porosity	VBM/CBM		E_g	
								Shortest	Largest		Wall	Base	Wall	Base
		Si	H	Total	[nm]	[nm]	[nm]	[nm]	[nm]	[%]	[eV]	[eV]	[eV]	[eV]
Pillar Diameter	1	1184	624	1808	7	1	**1**	2.17	3.46	93	-5.90 / -3.27	-5.22 / -3.63	2.63	1.59
	2	1834	824	2658	7	1	**2**	1.38	2.69	70	-5.54 / -3.64	-5.24 / -3.88	1.90	1.36
	3	3136	1016	4152	7	1	**3**	0.38	1.92	33	-5.26 / -3.73	-5.19 / -3.79	1.23	1.23
Pillar Height	1	237	100	337	**1**	1	1	0.54	1.15	70	-5.50 / -2.91	-5.02 / -3.57	2.59	1.45
	2	866	576	1442	**10**	1	1	0.54	1.15	70	-5.61 / -3.06	-5.08 / -3.72	2.55	1.36
	3	1532	1080	2612	**20**	1	1	0.54	1.15	70	-5.59 / -3.03	-5.09 / -3.75	2.56	1.34
	4	2235	1612	3847	**30**	1	1	0.54	1.15	70	-5.53 / -3.00	-5.08 / -3.76	2.53	1.32
	5	2901	2116	5017	**40**	1	1	0.54	1.15	70	-5.55 / -3.04	-5.09 / -3.77	2.51	1.32
	6	3567	2620	6187	**50**	1	1	0.54	1.15	70	-5.51 / -2.97	-5.08 / -3.76	2.54	1.32
Base Layer	1	1184	624	1808	7	**1**	1	2.17	3.46	93	-5.90 / -3.27	-5.22 / -3.63	2.63	1.59
	2	1569	652	2221	7	**2**	1	2.17	3.46	93	-5.70 / -3.18	-4.95 / -3.58	2.52	1.37
	3	2145	652	2797	7	**3**	1	2.17	3.46	93	-5.56 / -3.16	-4.80 / -3.62	2.40	1.18
Interpillar Distance	1	468	400	868	10	1	1	**0.38**	0.77	33	-5.70 / -3.20	-5.22 / -3.94	2.50	1.28
	2	866	576	1442	10	1	1	**0.54**	1.15	70	-5.61 / -3.06	-5.08 / -3.73	2.55	1.35

Pillar diameter = 1 nm	3	1006	632	1638	10	1	1	**1.09**	1.92	83	-5.68 / -3.13	-5.07 / -3.73	2.55	1.34
	4	1186	704	1890	10	1	1	**1.63**	2.69	89	-5.77 / -3.26	-5.04 / -3.72	2.51	1.32
	5	1406	792	2198	10	1	1	**2.17**	3.46	93	-5.82 / -3.29	-5.00 / -3.67	2.53	1.33
	6	1666	896	2562	10	1	1	**2.71**	4.22	95	-5.82 / -3.39	-4.97 / -3.64	2.43	1.33
	7	1966	1016	2982	10	1	1	**3.26**	4.99	96	-5.81 / -3.43	-4.94 / -3.60	2.38	1.34
Pillar diameter = 1.5 nm	1	999	604	1603	10	1	1.5	**0.38**	1.15	33	-5.43 / -3.28	-5.19 / -3.71	2.15	1.48
	2	1111	660	1771	10	1	1.5	**0.86**	1.92	63	-5.43 / -3.23	-4.99 / -3.65	2.20	1.34
	3	1255	732	1987	10	1	1.5	**1.38**	2.69	76	-5.52 / -3.34	-5.06 / -3.62	2.18	1.44
	4	1431	820	2251	10	1	1.5	**1.92**	3.46	83	-5.49 / -3.42	-5.03 / -3.59	2.07	1.44
	5	1639	924	2563	10	1	1.5	**2.46**	4.22	88	-5.53 / -3.48	-4.99 / -3.56	2.05	1.43
	6	1879	1044	2923	10	1	1.5	**2.99**	4.99	91	-5.55 / -3.51	-4.96 / -3.52	2.04	1.44
	7	2151	1180	3331	10	1	1.5	**3.54**	5.76	93	-5.60 / -3.54	-4.92 / -3.48	2.06	1.44
	8	2455	1332	3787	10	1	1.5	**4.08**	6.53	94	-5.61 / -3.58	-4.90 / -3.45	2.03	1.45
Pillar diameter = 2 nm	1	1947	956	2903	10	1	2	**0.38**	1.15	33	-5.16 / -3.44	-5.13 / -3.65	1.75	1.48
	2	2091	1028	3119	10	1	2	**0.86**	1.92	57	-5.21 / -3.42	-5.09 / -3.63	1.79	1.46
	3	2267	1116	3383	10	1	2	**1.38**	2.69	70	-5.25 / -3.47	-5.06 / -3.62	1.78	1.44
	4	2475	1220	3695	10	1	2	**1.92**	3.46	78	-5.34 / -3.52	-5.03 / -3.60	1.82	1.43
	5	2715	1340	4055	10	1	2	**2.46**	4.22	83	-5.37 / -3.55	-5.00 / -3.56	1.82	1.44
	6	2987	1476	4463	10	1	2	**2.99**	4.99	87	-5.38 / -3.59	-4.97 / -3.54	1.79	1.43
	7	3291	1628	4919	10	1	2	**3.54**	5.76	89	-5.42 / -3.62	-4.95 / -3.51	1.80	1.44
c-Si	-	144	8	152	-	-	-	Bulk	Bulk	0	-	-5.03 / -3.96	1.07	

Table S4: Computed band gap (E_g) of the craters models, calculated by its valence band maximum (VBM) and conduction band minimum (CBM) (not shown in the table), along with its corresponding number of atoms, and pore features. The band gaps of the crater are divided into the wall and base parts, which are calculated separately to investigate the effect of the local band gap. Three key features are varied to investigate the effect of each part: crater depth crater wall thickness, and crater diameter.

Model Name		Number of Atom			Depth	Base	Crater Diameter	Thickest Wall	Thinnest Wall	Porosity	VBM/CBM		E_g	
											Wall	Base	Wall	Base
		Si	H	Total	[nm]	[nm]	[nm]	[nm]	[nm]	[%]	[eV]	[eV]	[eV]	[eV]
Crater Depth	1	1823	576	2399	**4**	1	2.4	1.92	0.86	34	-5.20 / -3.60	-5.08 / -3.69	1.63	1.45
	2	2491	784	3275	**6**	1	2.4	1.92	0.86	37	-5.18 / -3.57	-5.06 / -3.63	1.61	1.43
	3	3827	1200	5027	**10**	1	2.4	1.92	0.86	39	-5.18 / -3.55	-5.03 / -3.58	1.60	1.39
Crater Wall Thickness	1	1823	576	2399	4	1	2.4	**1.92**	0.86	34	-5.20 / -3.60	-5.08 / -3.69	1.60	1.39
	2	2759	680	3439	4	1	2.4	**2.69**	1.38	25	-5.04 / -3.77	-5.04 / -3.77	1.27	1.27
	3	3839	800	4639	4	1	2.4	**3.46**	1.92	19	-5.00 / -3.82	-5.00 / -3.82	1.18	1.18
Crater Diameter	1	895	348	1243	4	1	4	**0.38**	0	79	-6.85 / -2.38	-5.03 / -3.61	4.47	1.42
	2	989	392	1381	4	1	3.8	**0.77**	0	73	-6.41 / -3.21	-5.05 / -3.62	2.93	1.43
	3	1087	476	1563	4	1	3.5	**0.96**	0	64	-5.89 / -3.17	-5.07 / -3.55	2.72	1.52
	4	1137	444	1581	4	1	3.45	**1.15**	0	63	-5.69 / -3.49	-5.09 / -3.62	2.20	1.47
	5	1259	644	1903	4	1	3.2	**1.15**	0.12	56	-5.67 / -3.43	-5.10 / -3.58	2.24	1.52
	6	1525	608	2133	4	1	2.8	**1.54**	0.38	44	-5.31 / -3.55	-5.08 / -3.66	1.76	1.42
	7	1823	576	2399	4	1	2.4	**1.92**	0.86	34	-5.20 / -3.60	-5.08 / -3.69	1.60	1.39
c-Si	-	144	8	152	0	0	0	Bulk	Bulk	0	-	-5.03 / -3.96	1.07	