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Interplay between structural changes, surface states and quantum confinement effects in thin films of semiconducting Mg_2Si and Ca_2Si

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Supplementary materials

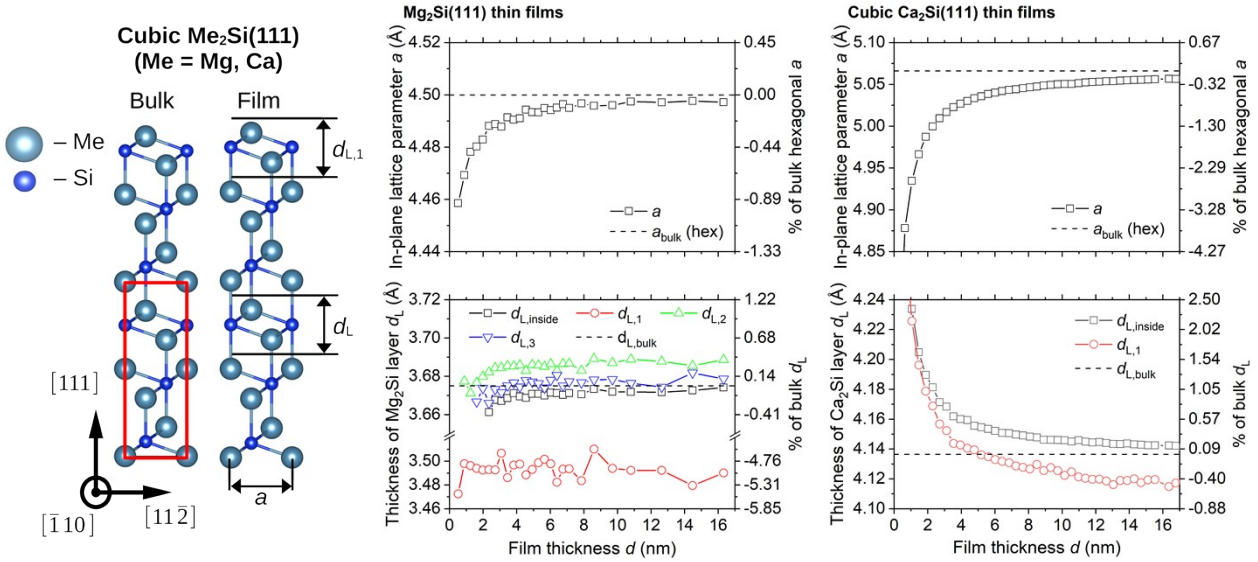

Fig. S1 Changes in the in-plane lattice parameters and interlayer distances (d_L) of cubic $Me_2Si(111)$ thin films. The corresponding film structures are also shown. $d_{L,1}$, $d_{L,2}$, …, $d_{L,inside}$ indicate surface, subsurface, …, middle or bulk-like layers, respectively. One bulk unit cell is indicated by a red rectangle.

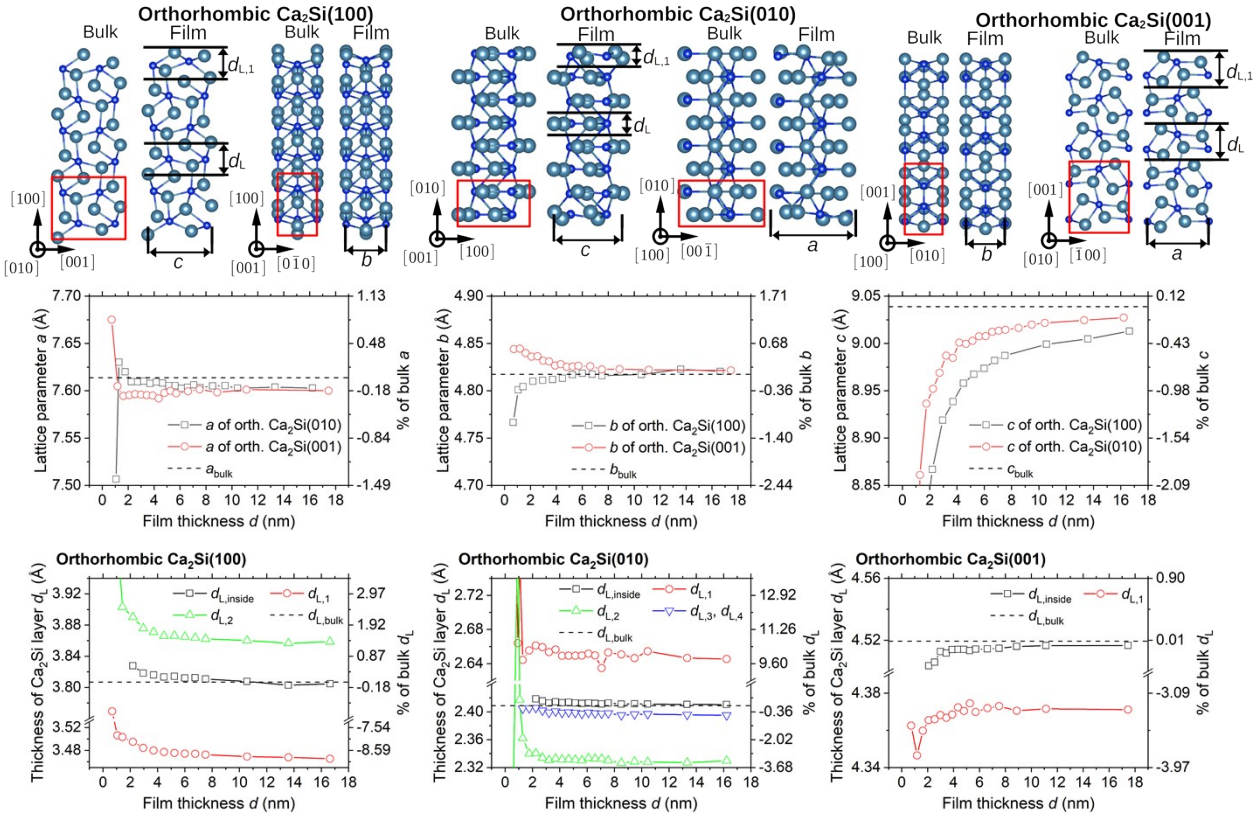

Fig. S2 Changes in the in-plane lattice parameters and interlayer distances (d_L) of orthorhombic $Ca_2Si(111)$ thin films. The corresponding film structures are also shown. $d_{L,1}$, $d_{L,2}$, …, $d_{L,inside}$ indicate surface, subsurface, …, middle or bulk-like layers, respectively. One bulk unit cell is indicated by a red rectangle.

Table T1. Structural information on atomic positions and lattice parameters of Me_2Si thin films shown in Figs. 1 and 2

Atom name	***x*, relative units**	***y*, relative units**	***z*, Å**
Cubic $Mg_2Si(111)$, d = 0.5 nm, a_{hex} = 4.458 Å			
Mg	0.0000	0.0000	0.000
Si	0.6667	0.3333	0.679
Mg	0.3333	0.6667	1.704
Mg	0.6667	0.3333	3.473
Si	0.3333	0.6667	4.497
Mg	0.0000	0.0000	5.176
Orthorhombic $Mg_2Si(001)$, d = 0.6 nm, a_{orth} = 6.899 Å, b_{orth} = 4.263 Å			
Mg	0.4894	0.2500	0.000
Si	0.2591	0.7500	0.176
Mg	0.8725	0.7500	0.528
Mg	0.1446	0.2500	1.665
Si	0.7578	0.2500	1.967
Mg	0.4765	0.7500	2.492
Mg	0.9765	0.7500	3.766
Si	0.2578	0.2500	4.292
Mg	0.6446	0.2500	4.593
Mg	0.3725	0.7500	5.730
Si	0.7591	0.7500	6.083
Mg	0.9894	0.2500	6.259
Cubic $Mg_2Si(111)$, d = 2.0 nm, a_{hex} = 4.483 Å			
Mg	0.0000	0.0000	0.000
Si	0.6667	0.3333	0.684
Mg	0.3333	0.6667	1.686
Mg	0.6667	0.3333	3.492
Si	0.3333	0.6667	4.431
Mg	0.0000	0.0000	5.350
Mg	0.3333	0.6667	7.188
Si	0.0000	0.0000	8.106
Mg	0.6667	0.3333	9.025
Mg	0.0000	0.0000	10.861
Si	0.6667	0.3333	11.780
Mg	0.3333	0.6667	12.697
Mg	0.6667	0.3333	14.536
Si	0.3333	0.6667	15.455
Mg	0.0000	0.0000	16.393
Mg	0.3333	0.6667	18.200
Si	0.0000	0.0000	19.201
Mg	0.6667	0.3333	19.886
Cubic $Ca_2Si(111)$, d = 2.3 nm, a_{hex} = 4.999 Å			
Ca	0.0000	0.0000	0.000
Si	0.6667	0.3333	1.014
Ca	0.3333	0.6667	2.092
Ca	0.6667	0.3333	4.169
Si	0.3333	0.6667	5.223
Ca	0.0000	0.0000	6.276

Ca	0.3333	0.6667	8.350
Si	0.0000	0.0000	9.401
Ca	0.6667	0.3333	10.455
Ca	0.0000	0.0000	12.531
Si	0.6667	0.3333	13.585
Ca	0.3333	0.6667	14.636
Ca	0.6667	0.3333	16.710
Si	0.3333	0.6667	17.763
Ca	0.0000	0.0000	18.817
Ca	0.3333	0.6667	20.894
Si	0.0000	0.0000	21.972
Ca	0.6667	0.3333	22.986
Orthorhombic $Ca_2Si(100)$, d = 2.2 nm, a_{orth} = 4.810 Å, b_{orth} = 8.867 Å			
Ca	0.2500	0.8095	0.000
Ca	0.2500	0.4039	0.427
Si	0.7500	0.6153	1.089
Si	0.2500	0.1054	1.596
Ca	0.7500	0.9386	2.192
Ca	0.7500	0.3256	3.057
Ca	0.2500	0.6797	3.495
Ca	0.2500	0.0761	4.553
Si	0.7500	0.8894	5.233
Si	0.2500	0.3991	5.257
Ca	0.7500	0.5698	6.012
Ca	0.7500	0.1714	7.024
Ca	0.2500	0.8142	7.308
Ca	0.2500	0.4189	8.335
Si	0.7500	0.5958	9.053
Si	0.2500	0.0974	9.113
Ca	0.7500	0.9169	9.811
Ca	0.7500	0.3141	10.836
Ca	0.2500	0.6702	11.152
Ca	0.2500	0.0674	12.176
Si	0.7500	0.8869	12.874
Si	0.2500	0.3885	12.934
Ca	0.7500	0.5653	13.653
Ca	0.7500	0.1701	14.679
Ca	0.2500	0.8129	14.964
Ca	0.2500	0.4145	15.976
Si	0.7500	0.5852	16.731
Si	0.2500	0.0949	16.754
Ca	0.7500	0.9082	17.434
Ca	0.7500	0.3046	18.492
Ca	0.2500	0.6587	18.931
Ca	0.2500	0.0457	19.795
Si	0.7500	0.8788	20.391
Si	0.2500	0.3690	20.899
Ca	0.7500	0.5804	21.561
Ca	0.7500	0.1748	21.987
Orthorhombic $Ca_2Si(010)$, d = 1.8 nm, a_{orth} = 8.936 Å, b_{orth} = 7.620 Å			

Ca	0.3845	0.1324	0.000
Ca	0.1155	0.6324	0.000
Si	0.0827	0.2525	0.473
Si	0.4173	0.7525	0.473
Ca	0.8152	0.0297	0.706
Ca	0.6848	0.5297	0.706
Si	0.6002	0.2441	2.655
Si	0.8998	0.7441	2.655
Ca	0.3249	0.4795	2.681
Ca	0.1751	0.9795	2.681
Ca	0.9295	0.3528	2.869
Ca	0.5705	0.8528	2.869
Ca	0.4226	0.1565	5.173
Ca	0.0774	0.6565	5.173
Ca	0.8243	0.0210	5.225
Ca	0.6757	0.5210	5.225
Si	0.1042	0.2554	5.261
Si	0.3958	0.7554	5.261
Si	0.6034	0.2483	7.588
Si	0.8966	0.7483	7.588
Ca	0.3210	0.4822	7.614
Ca	0.1790	0.9822	7.614
Ca	0.9250	0.3490	7.634
Ca	0.5750	0.8490	7.634
Ca	0.4250	0.1568	10.028
Ca	0.0750	0.6568	10.028
Ca	0.8210	0.0236	10.049
Ca	0.6790	0.5236	10.049
Si	0.1034	0.2575	10.074
Si	0.3966	0.7575	10.074
Si	0.6042	0.2504	12.402
Si	0.8958	0.7504	12.402
Ca	0.3243	0.4848	12.438
Ca	0.1757	0.9848	12.438
Ca	0.9226	0.3493	12.490
Ca	0.5774	0.8493	12.490
Ca	0.4295	0.1530	14.794
Ca	0.0705	0.6530	14.794
Ca	0.8249	0.0264	14.981
Ca	0.6751	0.5264	14.981
Si	0.1002	0.2617	15.007
Si	0.3998	0.7617	15.007
Ca	0.3152	0.4761	16.956
Ca	0.1848	0.9761	16.956
Si	0.5827	0.2533	17.190
Si	0.9173	0.7533	17.190
Ca	0.8845	0.3734	17.663
Ca	0.6155	0.8734	17.663
Orthorhombic $Ca_2Si(001)$, d = 2.1 nm, a_{orth} = 7.595 Å, b_{orth} = 4.837 Å			
Ca	0.7731	0.5000	0.000

Si	0.9817	0.0000	0.643
Ca	0.3741	0.0000	0.652
Ca	0.0958	0.5000	2.167
Si	0.4928	0.5000	2.268
Ca	0.7525	0.0000	3.027
Ca	0.2519	0.0000	4.366
Si	0.9878	0.5000	5.049
Ca	0.5837	0.5000	5.240
Ca	0.8921	0.0000	6.633
Si	0.4910	0.0000	6.866
Ca	0.2203	0.5000	7.560
Ca	0.7208	0.5000	8.839
Si	0.9915	0.0000	9.528
Ca	0.3940	0.0000	9.771
Ca	0.0841	0.5000	11.133
Si	0.4866	0.5000	11.376
Ca	0.7573	0.0000	12.064
Ca	0.2578	0.0000	13.343
Si	0.9871	0.5000	14.037
Ca	0.5860	0.5000	14.270
Ca	0.8944	0.0000	15.663
Si	0.4903	0.0000	15.855
Ca	0.2262	0.5000	16.538
Ca	0.7256	0.5000	17.876
Si	0.9854	0.0000	18.635
Ca	0.3824	0.0000	18.736
Ca	0.1040	0.5000	20.252
Si	0.4964	0.5000	20.260
Ca	0.7050	0.0000	20.903

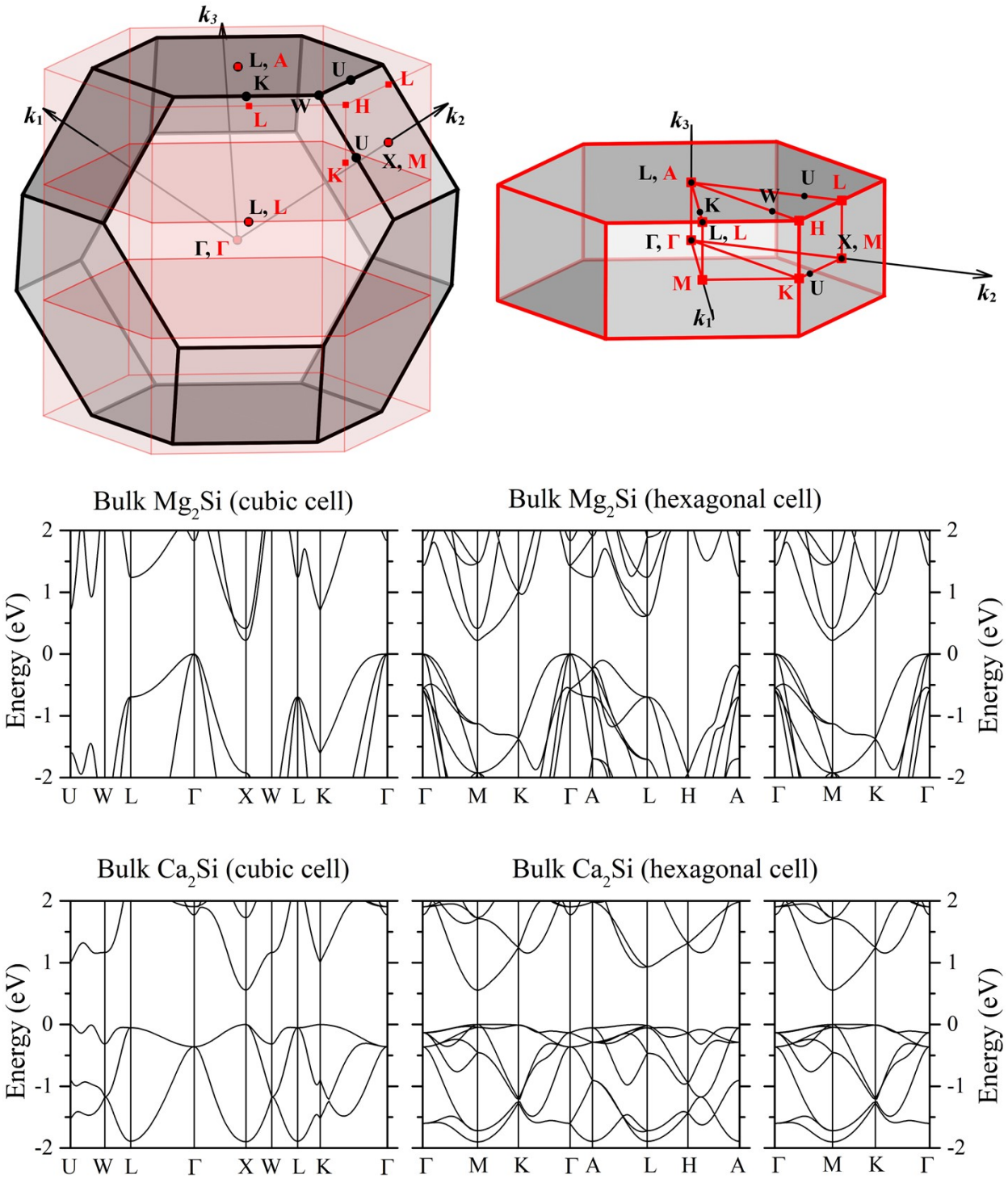

Fig. S3 The corresponding Brillouin zones and band structures of Me_2Si bulks represented by face-centered cubic and hexagonal symmetries. For the sake of comparison the face-centered cubic Brillouin zone (top left) is merged with its equivalent hexagonal representation. The high symmetry points of the Brillouin zones labelled in black and in red correspond to face-centered cubic and hexagonal symmetries, respectively.