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Electronic Supplementary Information

The influence of Ca-Mg disorder on the growth of dolomite. A computational study

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Table S1 Energy per formula units (eV/f.u.) of the optimized $n(10.4)^{i}_{Dol}$ slabs, $e^{i,n}_{Dol}$; i = R1, R2, R3.

		$e^{i,n}_{Dol}$			
layer (n)	R1	R2	R2-R1	R3	R3-R1
1	-86,25994715	-86,22906949	0,03087765	-86,24046445	0,01948270
2	-87,18205107	-87,23702695	-0,05497589	-87,24511911	-0,06306804
3	-87,46853359	-87,41549150	0,05304210	-87,44765091	0,02088269
4	-87,68206562	-87,59975083	0,08231479	-87,64221677	0,03984884
6	-87,87694867	-87,79261170	0,08433697	-87,84024174	0,03670693
8	-87,97845132	-87,89336712	0,08508420	-87,94272979	0,03572153
10	-88,04054474	-87,95454054	0,08600420	-88,00504079	0,03550395
12	-88,08229137	-87,99593854	0,08635284	-88,04682504	0,03546633
14	-88,11227219	-88,02548869	0,08678350	-88,07718992	0,03508227
16	-88,13483001	-88,04775558	0,08707444	-88,09980331	0,03502670
18	-88,15241550	-88,06512940	0,08728611	-88,11742846	0,03498704
20	-88,16650739	-88,07898007	0,08752732	-88,13155040	0,03495699
30	-88,20891269	-88,12101339	0,08789930	-88,17402137	0,03489132

Table S2 Energy per formula units (eV/f.u.) of the optimized $n(10.4)^{i}_{Dol}$ slab in epitaxial contact with the $m(10.4)_{Cal}$ slab, $e^{i}_{(n,m)}$; n = number of 10.4 layers of dolomite; m = number of 10.4 layers of calcite; i = R1, R2, R3.

$e^{i}_{(1,m)}$					
layer (m)	R1	R2	R2-R1	R3	R3-R1
3	-86,79314760	-86,76958983	0,02355776	-86,78015368	0,01299392
8	-86,74660384	-86,71972969	0,02687415	-86,73291468	0,01368916
14	-86,70405509	-86,63495790	0,06909719	-86,69059060	0,01346449
20	-86,66852653	-86,62232033	0,04620620	-86,64932745	0,01919908
30	-86,63773604	-86,61551108	0,02222496	-86,65916835	-0,02143231
40	-86,62527863	-86,61255912	0,01271951	-86,65394726	-0,02866863
50	-86,62562398	-86,60966370	0,01596028	-86,64451852	-0,01889455

$e^{i}_{(2,m)}$					
layer (m)	R1	R2	R2-R1	R3	R3-R1
3	-87,57860612	-87,46993905	0,10866707	-87,53714570	0,04146043
8	-87,53358373	-87,44278854	0,09079519	-87,48619258	0,04739115
14	-87,49424436	-87,42879757	0,06544679	-87,44146482	0,05277954
20	-87,47216260	-87,40350238	0,06866022	-87,42174804	0,05041457
30	-87,40878120	-87,39180683	0,01697437	-87,37862880	0,03015240
40	-87,38578311	-87,38577280	0,00001030	-87,37159283	0,01419027
50	-87,37783539	-87,38244812	-0,00461273	-87,36751424	0,01032115

$e^{i}_{(3,m)}$					
layer (m)	R1	R2	R2-R1	R3	R3-R1
3	-87,79632547	-87,71493920	0,08138626	-87,76259990	0,03372556
8	-87,74104827	-87,65421738	0,08683089	-87,70611490	0,03493337
14	-87,70427718	-87,61480012	0,08947707	-87,66925197	0,03502521
20	-87,64943434	-87,57225269	0,07718165	-87,64658662	0,00284772
30	-87,62146684	-87,57377840	0,04768844	-87,58439087	0,03707597
40	-87,60618923	-87,56656010	0,03962913	-87,56967196	0,03651727
50	-87,59659663	-87,56237033	0,03422630	-87,56126997	0,03532666

$e^{i}_{(4,m)}$					
layer (m)	R1	R2	R2-R1	R3	R3-R1
3	-87,93318538	-87,84673130	0,08645408	-87,89645238	0,03673299
8	-87,89568804	-87,80111451	0,09457354	-87,85681736	0,03887068
14	-87,86282784	-87,76070159	0,10212625	-87,82293755	0,03989029
20	-87,84116957	-87,74310421	0,09806536	-87,80229452	0,03887505
30	-87,81757837	-87,70392742	0,11365095	-87,77738702	0,04019136
40	-87,76166794	-87,69119591	0,07047203	-87,71925913	0,04240881
50	-87,74982510	-87,68470018	0,06512492	-87,70825065	0,04157445

Table S3 Potential energies (eV) of the optimized $n^{(10.4)}{}^{i}_{Dol}$ slabs in epitaxy with $m^{(10.4)}{}_{Cal}$ slabs, $E^{\ i}_{(n,m)}$; n = number of 10.4 layers of dolomite; m = number of 10.4 layers of calcite; i = R1, R2, R3.

$E^{\ i}_{(1,m)}$			
layer (m)	R1	R2	R3
3	-263,71519435	-263,61578099	-263,66821983
8	-263,79372666	-263,70458325	-263,74298212
14	-264,06479874	-263,93793509	-264,02046617
20	-264,01271043	-263,92060745	-263,96106776
30	-263,98510920	-263,92359531	-263,99039334
40	-263,96880565	-263,92116077	-263,98360615
50	-263,96790548	-263,91823894	-263,97524215

$E^{\ i}_{(2,m)}$			
layer (m)	R1	R2	R3
3	-528,39888016	-527,98367894	-528,16190296
8	-528,45305268	-528,08875752	-528,19352420
14	-528,63401582	-528,45616441	-528,37332326
20	-528,50804125	-528,39717591	-528,32539457
30	-528,30463528	-528,37908137	-528,28606207
40	-528,23644105	-528,36441130	-528,26970991
50	-528,20811736	-528,35496861	-528,25919825

$E^{\ i}_{(3,m)}$			
layer (m)	R1	R2	R3
3	-793,22223462	-792,43690411	-792,89970892
8	-792,87555420	-792,09658022	-792,53955661
14	-792,98547226	-792,25610829	-792,65022650
20	-792,72670498	-792,08816693	-792,48442611
30	-792,59755321	-792,16905438	-792,26083231
40	-792,52256454	-792,13754062	-792,19563308
50	-792,47035839	-792,11928897	-792,15113117

$E^{\ i}_{(4,m)}$			
layer (m)	R1	R2	R3
3	-1058,08100330	-1056,99170628	-1057,61337720
8	-1057,78270984	-1056,62609428	-1057,29799728
14	-1057,80010645	-1056,69393880	-1057,29985745
20	-1057,55322655	-1056,49413807	-1057,08649412
30	-1057,31325734	-1056,33415679	-1056,81393696
40	-1056,97786857	-1056,26031307	-1056,50029063
50	-1056,89796787	-1056,21849503	-1056,41936122

Table S4 Excess free energies (eV) of the optimized $n^{(10.4)}{}^{i}_{Dol}$ slab in epitaxy with $m^{(10.4)}{}_{Cal}$ slabs, related to the formation of the dolomite/vacuum surface and dolomite/calcite interface, $\varphi^{i}_{(n,m)}$; n = number of 10.4 layers of dolomite; m = number of 10.4 layers of calcite; i = R1, R2, R3.

$\varphi^{i}_{(1,m)}$			
layer (m)	R1	R2	R3
3	1,15180565	0,89421902	1,02178018
8	1,07327334	0,80541675	0,94701789
14	0,80220126	0,57206491	0,66953383
20	0,85428957	0,58939255	0,72893224
30	0,88189080	0,58640469	0,69960666
40	0,89819435	0,58883923	0,70639385
50	0,89909452	0,59176106	0,71475785

$\varphi^{i}_{(2,m)}$			
layer (m)	R1	R2	R3
3	1,33511984	1,03632107	1,21809704
8	1,28094732	0,93124248	1,18647580
14	1,09998418	0,56383559	1,00667674
20	1,22595875	0,62282409	1,05460543
30	1,42936473	0,64091863	1,09393793
40	1,49755896	0,65558870	1,11029009
50	1,52588264	0,66503139	1,12080175

$\varphi^{i}_{(3,m)}$			
layer (m)	R1	R2	R3
3	1,37876538	1,09309589	1,17029109
8	1,72544581	1,43341978	1,53044339
14	1,61552774	1,27389171	1,41977350
20	1,87429503	1,44183307	1,58557390
30	2,00344679	1,36094563	1,80916769
40	2,07843546	1,39245938	1,87436692
50	2,13064161	1,41071103	1,91886883

$\varphi^{i}_{(4,m)}$			
layer (m)	R1	R2	R3
3	1,38699671	1,04829372	1,14662280
8	1,68529016	1,41390572	1,46200272
14	1,66789355	1,34606120	1,46014255
20	1,91477345	1,54586193	1,67350588
30	2,15474266	1,70584321	1,94606304
40	2,49013143	1,77968693	2,25970937
50	2,57003213	1,82150497	2,34063878

Table S5 The adhesion energies (J/m^2) of the optimized $n{(10.4)}_{Dol}^{i}$ slabs in epitaxy with m ${(10.4)}_{Cal}$ slabs, $\beta_{(n,m)}^{i}$; n = number of 10.4 layers of dolomite; m = number of 10.4 layers of calcite; i = R1, R2, R3.

$\beta_{(1,m)}^{i}$			
layer (m)	R1	R2	R3
3	0,68358045	0,68265076	0,68520060
8	0,68501903	0,68133103	0,68575710
14	0,71356175	0,70359684	0,71580553
20	0,70143682	0,69790633	0,70129747
30	0,69412954	0,69656820	0,70187887
40	0,69068385	0,69551247	0,69987051
50	0,69031988	0,69472816	0,69825821

$\beta_{(2,m)}^{i}$			
layer (m)	R1	R2	R3
3	0,74513237	0,63242159	0,65826946
8	0,74191931	0,63943450	0,65250681
14	0,75925596	0,68108984	0,66992270
20	0,73805624	0,66619385	0,65822927
30	0,69947454	0,66112316	0,64283481
40	0,68709028	0,65798814	0,63927103
50	0,68232043	0,65610030	0,63714913

$\beta_{(3,m)}^{i}$			
layer (m)	R1	R2	R3
3	0,84773489	0,80586557	0,82942419
8	0,78651803	0,74379076	0,76604523
14	0,79307120	0,75519133	0,77296748
20	0,74460703	0,72005134	0,74554639
30	0,72266267	0,72632548	0,70242127
40	0,71031693	0,72035768	0,69132242
50	0,70197371	0,71689590	0,68407028

$\beta_{(4,m)}^{i}$			
layer (m)	R1	R2	R3
3	0,83554538	0,82288446	0,83806947
8	0,78245317	0,75876599	0,78158490
14	0,77634484	0,75715970	0,77332330
20	0,73746682	0,72499257	0,73915736
30	0,70001580	0,69065123	0,69711504
40	0,64376252	0,67781817	0,64342514
50	0,63136875	0,67077623	0,63093196