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SUPPORTING INFORMATION

For "*Role of nano amorphous interface in crystallization of Sb_2Te_3 towards nonvolatile phase change memory: insights from first principles*"

I. Supercell Parameters

Table S1. Lattice parameter of *b*-Si, *b*-ST and *i*-ST

	a (Å)	b (Å)	c (Å)	α	β	γ
***b*-Si**	**8.528**	**8.528**	**30.458**			
***b*-ST**	**8.528**	**8.528**	**30.458**	**90 °**	**90 °**	**120 °**
***i*-ST**	**17.3875**	**8.5943**	**30.458**			

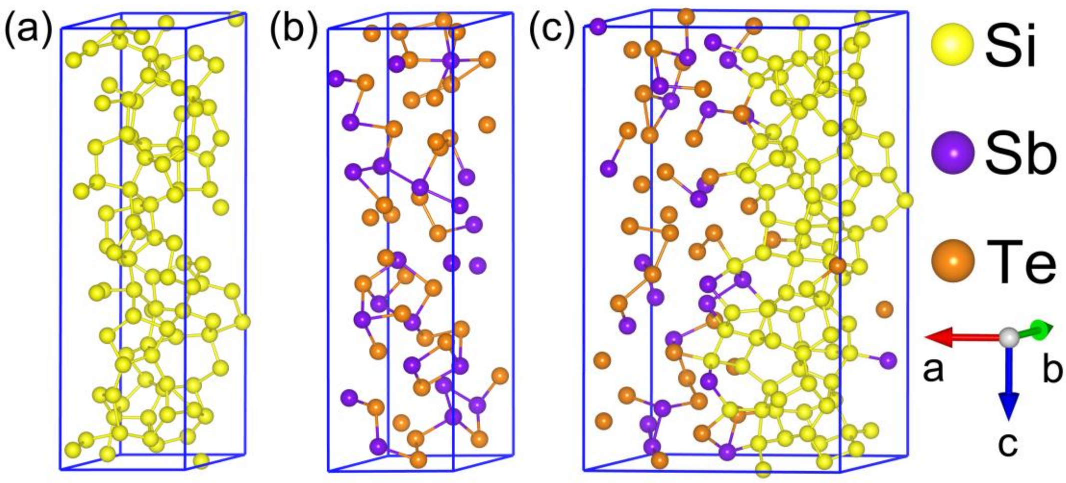

Fig. S1. Structure for (a) *b*-Si, (b) *b*-ST and (c) *i*-ST.

POSCAR Files containing atomic coordinates for *b*-Si, *b*-ST, and *i*-ST

***b*-Si:**

Lattice:
7.3854646503521604 -4.2640000039712804 0.0000000000000000

0.0000000000000010	8.5280000079425609	-0.0000000000000070
0.0000000000000200	0.0000000000000270	30.4580000283670991

Si

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Direct:

0.4868225012723833	0.1449450737757250	0.4445987046977511
0.3297013589892593	0.9499585968018049	0.6105477768050587
0.2499805282607520	0.2248335173052239	0.8830675529239330
0.7356657205928557	0.6137309568114382	0.2662570691300077
0.4524486046000338	0.3642553366730446	0.9421576890549834
0.4993085166694378	0.4464240543228044	0.0733742473002729
0.9145839277937935	0.0311580884800933	0.0730597730112886
0.6219923359129332	0.9113637161905771	0.1068097546645271
0.2619658418130273	0.4342421002433566	0.3804352209939474
0.9752342102646168	0.9651426513156418	0.8847846284177501
0.9110605834923501	0.0260631481009486	0.9561526029778021
0.3512752893545826	0.8943155737750806	0.0867338731463154
0.7600441983048438	0.8879181170896333	0.2958674643930223
0.6930176798290119	0.6026226187981920	0.1861446983566386
0.8871131929765455	0.5392585407016808	0.5116006926154452
0.4635022515628081	0.8978622590635164	0.2241541698047022
0.1421712243245777	0.1172726480008882	0.3808902701391503
0.8856799234616556	0.8566937984723059	0.7695129617002335
0.5903108953821579	0.0428768986127255	0.5091843762835517
0.0805412646640513	0.9976505469107527	0.0127846159367596
0.4154273111255265	0.3082608623991933	0.7510120288575072
0.0183448853342010	0.1424400008746018	0.2648702272520899
0.5367266668685354	0.6250507231499641	0.6559582331337817
0.7689351634413282	0.8042031516185900	0.4296745855712030
0.1658176092621265	0.1571228396980627	0.4918939655254356
0.0693696726988837	0.2622856329017650	0.5944701100939709
0.9090570710494398	0.4762231958164757	0.8468411793059212
0.2745067883285849	0.4440660134720640	0.2994432752743745
0.3754156880219842	0.0460821408275224	0.0203920853159466
0.1763135537715406	0.9541841311179357	0.4385405623058777
0.0307731584308762	0.8413122108396517	0.6244584769254488
0.2153459427430641	0.0625534219548615	0.3100590288909176
0.9144519737210483	0.5370449911309929	0.6119263164792393
0.1755782836616352	0.7684595922487604	0.7199283729855851
0.4005030791204414	0.8035526068510622	0.5587041391855697
0.2343784976499502	0.4483434991252872	0.6554159857573860
0.6282285597039911	0.2180751297764924	0.9241458762805815
0.9426484454258827	0.3135124315103638	0.9432639697865108
0.7579820093656744	0.1017222359622562	0.6031291429736573

0.3634415211325270	0.8934353538722200	0.8394988246525449
0.4867553688852743	0.8541516585819269	0.7278960513687297
0.1134385697826716	0.5061759420520595	0.9980543881382877
0.5579714775854288	0.1827996228229036	0.2461869412993311
0.9114468818046694	0.3048629804177484	0.0554077280893425
0.5925983394066345	0.6218760874630247	0.9036733104794960
0.5096934269064116	0.6983346915437046	0.8401380047003935
0.4389292474980007	0.4024079787028441	0.4882502846692278
0.0194850151923451	0.4975979365502107	0.6806965114478822
0.8665126425009254	0.7899216839018574	0.5480780380228452
0.8486691193765610	0.9887838169667907	0.4948574422278237
0.2051790786312861	0.7774795855824163	0.3231551889157100
0.8458572909609225	0.2881306071969096	0.3584103483163748
0.4984966501860227	0.1715257293597143	0.6574578635325330
0.6058974001470909	0.4051882719291809	0.6060347845120614
0.1754612513907234	0.0716001862880710	0.5663411185096222
0.1605824332190973	0.7124593542653113	0.2036144135559996
0.0806695585357765	0.0590208495788063	0.1367606080891443
0.6041629170002335	0.3041585640854470	0.1716998154188889
0.1144616175418023	0.5263125208821717	0.5529812537379124
0.6031747292549152	0.3143364371415095	0.5323393272818480
0.7922636140193426	0.5461218638400166	0.0490004485154853
0.4539740472681993	0.7650092919962953	0.2910928281345349
0.1906809352088928	0.5060065064008166	0.1646567672764390
0.6087113447963473	0.7895689061106890	0.9701917593920204
0.8616685971383491	0.2924543453125726	0.2790692742684973
0.6030857189641253	0.6362229817587741	0.7385110803471160
0.6721982255010382	0.2785892144191586	0.0074921921193313
0.9775454093444488	0.7596633564206571	0.1549559746817472
0.3338703774486452	0.3887877576599156	0.8191224293190743
0.8857675859335343	0.6619646559425385	0.9037163151402972
0.2485239030651435	0.2170559693959945	0.6879775837920105
0.7419986578054966	0.9919695339068125	0.6726306463536715
0.0041243412938732	0.5956886157924581	0.2696490890728883
0.9508247800136048	0.6554608649718607	0.4414173823104483
0.0004139589054412	0.9494844169363778	0.6980211089027081
0.7892986167290812	0.9809428845468855	0.8293894749739305
0.4934068346140527	0.3490206784566537	0.3046676911266800
0.6627830935854491	0.1745148016691473	0.8365632404561519
0.8368953111800135	0.0033349077613183	0.3689229022349471
0.0817381038195205	0.5709528396903001	0.3846985795147984
0.9553418296819258	0.6944930883634087	0.9880929507100080
0.7079304119087306	0.0850432670782837	0.1723969444591673
0.3838906031121947	0.1730154394625678	0.1128345267520571

0.0650859045677314	0.7241624435148660	0.7946428510027369
0.4307397605521076	0.9381325820993850	0.9569202060806824
0.2037132500243931	0.7621507408528984	0.9047924738498895
0.6014362868798138	0.3216442966370838	0.3761298597546016
0.6361527166391728	0.7772351317262681	0.5896887137518011
0.0498883154147302	0.6041688828808377	0.1040259899125359
0.4048584939743593	0.5103013151843233	0.0058475767715567
0.5319589650090697	0.5222296946719014	0.4171237712409590
0.4785172753524179	0.5991746105962795	0.1345864291246076
0.0261450754810246	0.2149410159588029	0.1903385093250159
0.7477889521611040	0.2564538198873267	0.7048004136385532
0.1466997571618391	0.4545777036207922	0.8803691970215489
0.5587066473726952	0.1272815968707035	0.7662976233656619

***b*-ST:**

Lattice:

7.3854646503521604	-4.2640000039712804	0.0000000000000000
0.0000000000000010	8.5280000079425609	-0.0000000000000070
0.0000000000000200	0.0000000000000270	30.4580000283670991

Sb Te

24 36

Direct:

0.2678218808579194	0.9583715519760134	0.8851189605457540
0.8836531221043351	0.1783365041891440	0.3296227095197952
0.8169586187368719	0.1877668718399538	0.6637105825960830
0.9312571765902193	0.2341795253781002	0.2197621398925886
0.4128341558533804	0.3099914703521890	0.3695981243338415
0.1053858823125463	0.1951994108913949	0.5372407124433697
0.9590591568213621	0.0452696508759730	0.1139834224165025
0.5875997077483737	0.5415611960921275	0.6824716778618116
0.9589012765939223	0.7620702281814796	0.6483954877290807
0.4752728191314970	0.0517451524600948	0.0820013341890815
0.7861942233054493	0.4638410227083037	0.3255336849330959
0.2352551614716768	0.4894062173531334	0.8946156316372483
0.1466418272830557	0.4197044082302027	0.7774028567433205
0.2633820327895358	0.7718100207564745	0.3632279334668984
0.4625011084145869	0.8033723610920380	0.8340111141223641
0.9928892285094294	0.8727522243469906	0.3413582646464033
0.2212130456874272	0.8079134477300990	0.4717697603189700
0.6567787606499063	0.1185105767517732	0.9486348248268877
0.2685981872005388	0.5252969422189117	0.0911363666551143
0.0930876593005515	0.3075371615702656	0.4109246519881039
0.8611447492725329	0.0612957306402512	0.8361773604132190

0.2601567760810483	0.9501702192911733	0.5694885222563110
0.6783958859867086	0.4908209452671234	0.5401742187166443
0.3423442111062701	0.0267053351383065	0.7617336176561591
0.5596400961541810	0.5382463325360067	0.9453714086102992
0.0979498837602764	0.2697342152995394	0.0168479699567882
0.3111814968704694	0.4297481988821839	0.2840606459581639
0.9564275276012351	0.9675125335333348	0.4537107472250745
0.0084930985378137	0.7965836758785786	0.8134343554293869
0.8241865461972335	0.3657096207951583	0.0231655098393126
0.2733572634357783	0.6993312155880895	0.7041720370532296
0.8250883662515345	0.8294890738523508	0.0359257515549966
0.8977146718815953	0.4944771390793868	0.4436369629026342
0.4680985277939138	0.1291562508003859	0.6482316263702286
0.1008285924265555	0.7776217394902696	0.0981302235583252
0.0232288942701108	0.6146824435592433	0.2396269700501895
0.1550585504276741	0.0418166997934212	0.2573502503091488
0.8643743082362914	0.9354875294752950	0.9236215743344686
0.5783746729362085	0.6481937385173291	0.4036942514802550
0.9512518403644805	0.4825905829767054	0.5929084320623506
0.4197016721067076	0.8463409130606807	0.1557073793020461
0.5798838534929371	0.0621014267165518	0.4008132324551699
0.1203834798501534	0.1327466279567857	0.7131511819243820
0.7784192387895829	0.3319922224198382	0.8674593667054313
0.8643829235518302	0.3449022679640495	0.1337076288043322
0.4198935672999684	0.8159287031206048	0.2765306764199102
0.8272804822507400	0.9316492987257899	0.5907485053603249
0.4526631151136185	0.7877931200693599	0.0108194721330274
0.3942452738613051	0.4908648130899740	0.6031480193234502
0.2966437875839355	0.3120184452128173	0.1678031249650140
0.4016902186683380	0.5825983608668632	0.4832968846505223
0.7813419665885670	0.3784080545545217	0.7418530130927888
0.1235898695186407	0.6918517874582510	0.9526313656363673
0.7279240614040892	0.8248327222735641	0.1905924169603150
0.5819359560553358	0.4902671323221440	0.0879448010555132
0.6361646518800465	0.8584870057696702	0.7290503824965719
0.6435615783380837	0.3562845813097179	0.2390496498262083
0.3660924471208940	0.1809042551427804	0.9806737058983552
0.5892075820322709	0.1090763904702677	0.5214867130636225
0.4113676550387239	0.3330677240482439	0.8227067419046420

***i*-ST:**

Lattice:

15.0580173690268992 -8.6937503814697195 0.0000000000000000

0.0000000000000000	8.5943002700805700	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.4580001831055007

Si Sb Te
96 24 36
Direct

0.4483927125776424	0.5190527583477721	0.2758881067683868
0.2400734366784287	0.6924512837995171	0.6427604209357805
0.1482434661278541	0.4960058096597674	0.4623604043562132
0.3672133408454040	0.8626396125392254	0.8972644062387626
0.0445842033322622	0.4111326950343138	0.9631062078661609
0.3194114679529899	0.1321196226876931	0.6386416393383709
0.0013157643145491	0.9654283424526849	0.4236213889810188
0.3638019418807463	0.7530202036234022	0.2058190403426415
0.1694560545715788	0.3655172430237872	0.6232879717381578
0.3896507600814639	0.1392837333911969	0.0657167242986630
0.1438972458481419	0.6882607321205124	0.7574682145638859
0.2971910276498942	0.8544866720980137	0.0992034420420330
0.1176413054569615	0.2510111303715060	0.8594547564826017
0.4130942269199724	0.5295162734175944	0.8309150696510510
0.1362443163992449	0.7472277123599145	0.4904781806996772
0.4379243422777146	0.7045820774885303	0.8879615293923959
0.0889193732829994	0.6231310135246277	0.5603147123860194
0.2855959230569833	0.3385270536421711	0.2738375472815199
0.1488795639101710	0.0724216846761837	0.5900820417049638
0.4453368270539989	0.4557913739502621	0.7156689675787029
0.3049918695013856	0.9936884624081489	0.4063855100603055
0.1988445676677398	0.2754368105360718	0.9236309637228441
0.4853097262398525	0.4147166765524971	0.3388020065443541
0.5335115968261180	0.5701854350908203	0.7836907057407383
0.1456742081721409	0.4145926114742359	0.5420394503727796
0.5987499710212163	0.3682080412375028	0.7644873340883621
0.1115550843862640	0.2864513701276083	0.7012238163309129
0.3185815731138393	0.0745686233406516	0.9981635822806431
0.2869195854582025	0.9349708925965357	0.5277856347994607
0.4433660329557016	0.9047158262206046	0.3311551810245386
0.2893899268268245	0.7173191553953119	0.4313646222491686
0.3091096049710265	0.5951121409031603	0.0106501288338837
0.5385202249804394	0.3457817117572378	0.6938553815884237
0.0104087177330637	0.2702686163083137	0.1064743766362179
0.3709807305905248	0.2691727787113081	0.5166642275763774
0.0325168612582670	0.8392877737297727	0.3611284773072270
0.5152488724033889	0.3955734224064643	0.5517149930712926
0.3377547514989441	0.7286136800188832	0.5065459435218523
0.4733461167403804	0.8052400333943227	0.2652087230307102

0.4663711143046117	0.1408404554344262	0.8660808370433351
0.2172658026056883	0.7461911510286603	0.8653096990723371
0.1417321616594216	0.0742276794111454	0.8030421039968938
0.3177228693208842	0.6003345036685911	0.0916494003527399
0.1871627876545296	0.4388463475177284	0.1460865926634348
0.0424071745333175	0.8434887829521421	0.2828026273706289
0.3951841282189011	0.2945862303293867	0.9471358295392237
0.3445185634751504	0.6445282328916191	0.3691760708043952
0.3471812587123488	0.5054889489787457	0.9435217670933348
0.0571228956824423	0.4683989630220194	0.1668140022927210
0.1517193736928769	0.7701307197345272	0.2621063683603366
0.3168197834212890	0.4074520554195272	0.6115383760960119
0.2232094773649769	0.2956863408589243	0.4584799149720815
0.2237784005112421	0.4359534425800362	0.3280799037012245
0.1044760111242275	0.1316212888872111	0.0366463338749464
0.2838952135890705	0.9057588220605178	0.1728218544543441
0.1170698244805991	0.5674178900540363	0.6872259423376076
0.1108546400502007	0.9968138367324244	0.4775326769702665
0.1935305756186861	0.9938496887543951	0.3653460634995082
0.3831472092167623	0.0910516110088673	0.3361292650972744
0.1290805682735415	0.9453805902835988	0.9412031902517553
0.4630482321853305	0.5150824214220610	0.1388217882798654
0.0420823709330741	0.2656401177881682	0.4149712834951234
0.3401395109257018	0.3329317018809287	0.0931317552508782
0.2586279390353106	0.0503267612692006	0.2955043622656318
0.1482221320797214	0.7356489608040447	0.0665040389857220
0.3094169748121118	0.1787053199711205	0.7115261688741238
0.2816152176999098	0.9579582926600021	0.7648565569157237
0.1691973489521564	0.5192464013748839	0.8155760851527702
0.4313808321160152	0.7464537393377418	0.1394735375314466
0.1320836325163085	0.7667672490660199	0.1866874015576184
0.0454284950125929	0.3092689950063660	0.2331252834971414
0.1715223383167327	0.9754396916579280	0.0160494921448406
0.4399546387687306	0.6138895036743793	0.6536791922703934
0.0343139419516083	0.4469298047415817	0.0429137952085549
0.2250442848934630	0.8914191161067293	0.5952280043388282
0.4144780237551254	0.4865969277526776	0.3891104350304476
0.3000058863900606	0.5431038099217281	0.7882910759509175
0.2940018068948092	0.8106373063326763	0.9661671856539870
0.2850834697806140	0.4199435576497323	0.5357099524698011
0.3505247215848786	0.2635647947137743	0.4408195702842139
0.2697664779403591	0.4202938872194151	0.2034313505642793
0.2944998560394468	0.2027884055281145	0.1656786623516304
0.2444221345243602	0.0197649925818146	0.8375581355209758

0.1260028600213331	0.0247703707266872	0.1681838432897856
0.0486789135147057	0.0469253662778470	0.2268612955669737
0.3707551747939775	0.2507290801271448	0.8699229693124811
0.1013857914247416	0.1603987917507593	0.1095228552292793
0.1486660489198828	0.6989883060220349	0.9363397477918951
0.2224793358936110	0.2966904649140743	0.7438370577476868
0.3674962412370595	0.8252434379807915	0.7539468224354946
0.3825877903552682	0.8089809115656312	0.6754343089271009
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0.4502214524357426	0.1102110050424378	0.6460837536540401
0.1703081824314241	0.2359672622778541	0.3861115697516493
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0.6163381550462774	0.6771637781011827	0.0988649012860792
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0.5483800197370581	0.1956437411710801	0.0412547077091275
0.7661606241351457	0.9108073502673629	0.3893329855945530
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0.9661786107322111	0.8269451375686656	0.9257195872867686
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0.5644831894757404	0.4726560740389646	0.9742343691311032
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0.9095084400337797	0.0247119352164253	0.3207659451366901
0.9031477769409429	0.6931801360466301	0.6349262061950924
0.8540181040511351	0.4585668221864255	0.9626960530555253
0.9222261740516526	0.5766762543847048	0.5526721125573528
0.9534576976860445	0.0338387272016007	0.0015379809226313
0.7167968650990655	0.0520660898894244	0.1346449318981505
0.5911603689521789	0.2003810383623526	0.9218327805598558
0.8700769056329904	0.1599215895654212	0.2398398677637356
0.7013237383027042	0.5714256526750801	0.8636509251099718
0.7216544700629975	0.8769513827832705	0.6929008125580750
0.9836481677427270	0.6529860116593210	0.0768380500371451
0.6151834410794143	0.4662900906271049	0.4806638000817507
0.5561954228406817	0.0791853269625949	0.1421391859107386

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0.8636006484150248	0.9468108680099784	0.1151035787133046
0.5304495144005456	0.7331518174603457	0.0245835283304107
0.7805385905647313	0.1861691968983433	0.5640372698258423
0.9057651914835561	0.1612193426503850	0.6289585903274693
0.9749844716622955	0.5427103301748890	0.8506863813700087
0.7151999507421432	0.0459810445942690	0.9776739164870546
0.9038833860793529	0.4938096923580046	0.3735192930341535
0.7075684213543135	0.0991840830019921	0.3302673108583601
0.7261730832959934	0.2385614640851692	0.4725736171941071
0.9681573202289395	0.1755183233163009	0.8950017442624909
0.9098075799657924	0.5377620753928593	0.1706941028521618
0.5091729403865463	0.9245176544903366	0.5122637219165627
0.6492583288778583	0.9040739891158863	0.7979675101361550
0.0196334143453487	0.0378701446964947	0.5359769810055205
0.7933939404310113	0.2433779627454965	0.0580838801078144
0.7538311182977393	0.4023713394880253	0.7473822603724901
0.4826525773975908	0.3718482642935206	0.2080730975747623
0.8549474577549273	0.7073477645683357	0.4493370340176474
0.6022245352584225	0.7652325195694095	0.9007066950971018
0.8360625737396126	0.9039786279223874	0.8244611782688029
0.8667180219237398	0.1739615655389772	0.4552648450876255
0.9760985146168596	0.1830674457498093	0.7586306008599688
0.7759190842743180	0.6613641157162105	0.0019478039059045
0.8937509188768173	0.5695215521899286	0.2654686212620270
0.5506316017218613	0.7417885595655124	0.4299711855728793
0.6672302106893651	0.3661688293233990	0.2646108561096584
0.7517223910812076	0.7348856715570131	0.5332213998650563
0.0734406378466709	0.9356785202888999	0.6681631946128685

II. No Magnetism for *b*-Si, *b*-ST and *i*-ST

We check the magnetic property of *b*-Si, *b*-ST and *i*-ST with spin calculation. As a result, the calculated magnetic moment of *b*-Si, *b*-ST and *i*-ST are all very small and are only -0.000005, -0.000012 and -0.000002 μ_B/atom, respectively, μ_B is for Bohr magneton here. In other words, the magnetism of *b*-Si, *b*-ST and *i*-ST can be neglected. Thus, the non-spin calculations in the main text are reasonable.

III. Definition of "Degree of Crystallization"

Our "degree of crystallization" is obtained on the base of the pair correlation functions (PCF) during the 36-ps crystallization of *i*-ST and *b*-ST. Here, we take *b*-ST as an example. First, we calculate every PCF averaged by 1000 steps for a special time stage, for example, the PCF at 12 ps is collected from 9~12 ps (1000 steps). Second, we choose the referenced distance at peaks and valleys in the PCF at final stage (36ps), shown by dash line in Fig. S2. Third, we calculate the average difference of $|g(t) - g(0ps)|$ at these referenced distances. Finally, normalization is based on the maximum (24 ps at *b*-ST) to watch the crystallization degree.

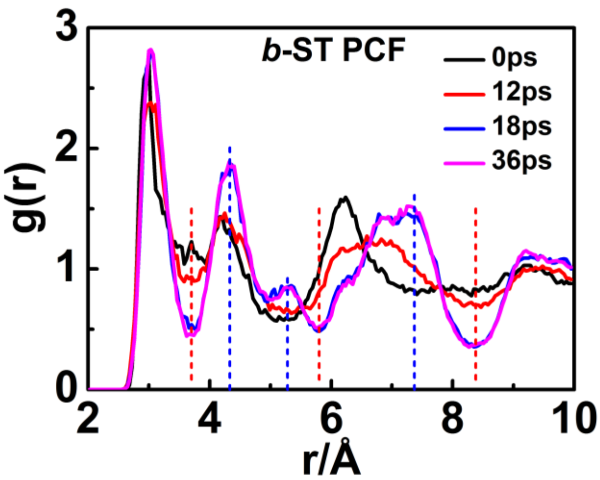

Fig. S2. PCF of *b*-ST during the 36-ps crystallization. The peaks (blue dash line) and valleys (red dash line) are the referenced distance for degree of crystallization.

IV. Amorphous Sb_2Te_3 Stability from Energetics

Fig. S3 displays the relative Helmholtz free energies extracted from *300K NVT AIMDs* for the amorphous Sb_2Te_3 models with/without interface pinning in the main text. It is clearly demonstrated that the Helmholtz free energy of interface amorphous Sb_2Te_3 is lower than that of bulk amorphous Sb_2Te_3. In other words, from energetics viewpoint, interface system can really enhance the stability of the amorphous Sb_2Te_3.

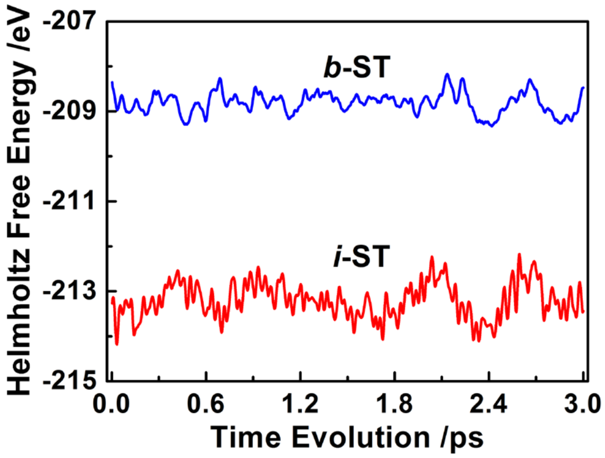

Fig. S3. Comparison of relative Helmholtz free energy at 300 K for different amorphous Sb_2Te_3 models in the main text: *b*-ST and *i*-ST. In the calculations of the interface model (parallel to *c* axis), the free energy of the part for Si has been subtracted according to that of bulk amorphous Si at 300 K.

V. Bond Angle Distribution of Si

Bulk amorphous Si (*b*-Si) is also obtained by the AIMD method. Fig. S4 shows bond angle distribution of Si in *i*-ST and *b*-Si, inset is the coordination number distribution. In both cases, Si displays the robust sp^3 bonding characteristic.

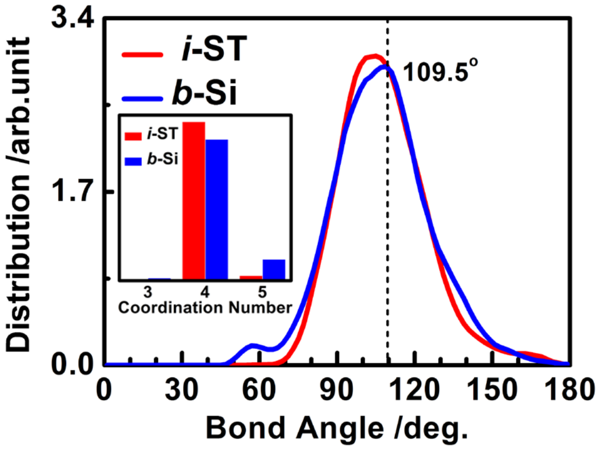

Fig. S4. Bond angle distribution and coordination number of Si in bulk amorphous Si (*b*-Si) and interface amorphous (*i*-ST) model.

VI. Electron Localization Function

As already stated in the main article, the electron localization degree of Sb_2Te_3 increases in *i*-ST according to the distribution of ELF=0.92. This conclusion remains valid if we select other high ELF values. Fig. S5 shows distribution of ELF=0.88 and ELF=0.9. Moreover, the distributions of the highly localized electrons also indicate in the form of a lone pair.

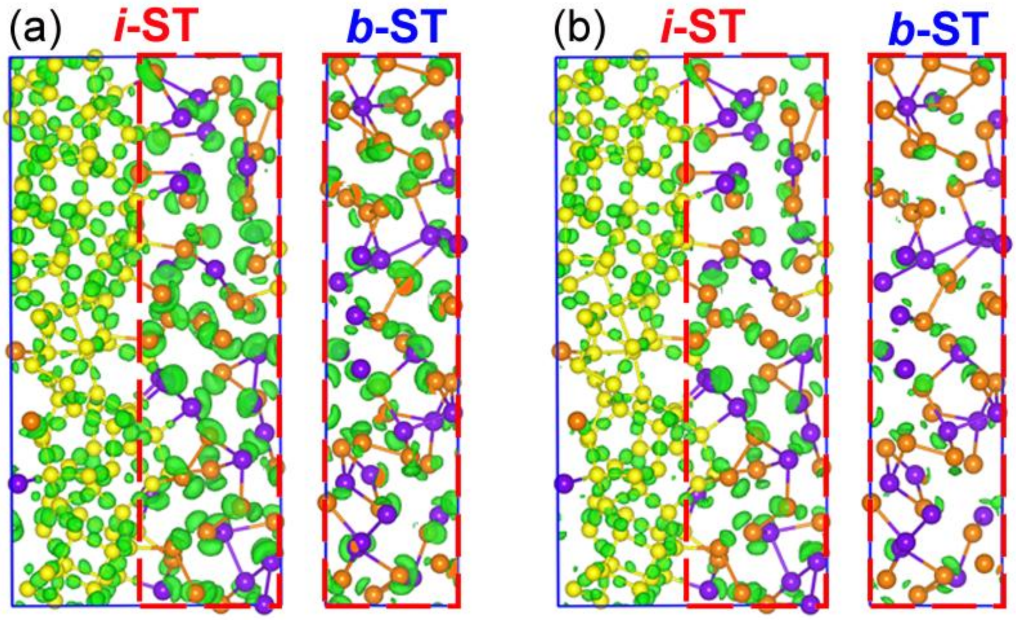

Fig. S5. Electron localization function of amorphous *i*-ST and *b*-ST, green area stands for the isosurface of (a) ELF=0.88 and (b) ELF=0.9.

VII. Model Effect: Different Interface Orientation

Compared to the original Sb_2Te_3 interface model [which is parallel to the *c* axis in the main text, *i*-ST (∥c)], another interface model [which is vertical to *c* axis in Fig. S6, *i*-ST (⊥c)] displays less distortion of Te local environment with the bond angle distribution closer to the bulk characteristic 90°. In fact, the "*i*-ST (⊥c)" model has shown a certain degree of crystallization according to one of the partial pair corresponding function. In other words, the interface-pinning effect on the amorphous stability of Sb_2Te_3 depends on the interface orientation, i.e. the interface *i*-ST (∥c) in the main text has much significant effects.

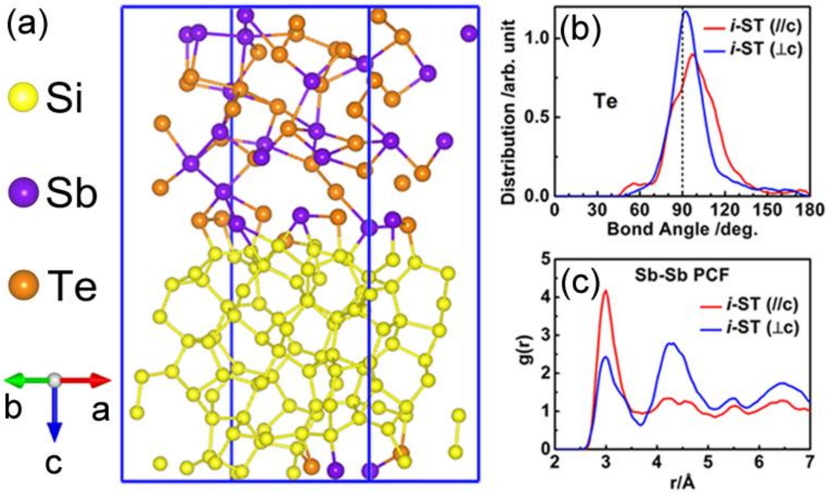

Fig. S6. (a) The new calculated structural model of the interface at 300 K which is vertical to *c* axis [*i*-ST (⊥c)]. In order to compare the one which is parallel to *c* axis in the main text [*i*-ST (//c)], (b) the bond angle distribution (BAD) around Te and (c) the pair corresponding function (PCF) of Sb-Sb are shown. Black dashed line in (b) highlights the prevailing bond angle of 90 °for bulk Sb_2Te_3.

VIII. Pseudopotential Information

Below are the information of the pseudopotentials for Si, Sb, and Te used in VASP code for the present studies.

Si:

```
PAW_GGA Si 05Jan2001
  4.00000000000000000
  parameters from PSCTR are:
    VRHFIN =Si: s2p2
    LEXCH = 91
    EATOM = 103.3076 eV, 7.5929 Ry
    TITEL = PAW_GGA Si 05Jan2001
    LULTRA =          F       use ultrasoft PP ?
    IUNSCR =          1       unscreen: 0-lin 1-nonlin 2-no
    RPACOR =      1.500       partial core radius
    POMASS =     28.085; ZVAL   =    4.000    mass and valenz
    RCORE  =      1.900       outmost cutoff radius
    RWIGS  =      2.480; RWIGS  =    1.312    wigner-seitz radius (au A)
    ENMAX  =    245.435; ENMIN  =  184.076 eV
    ICORE  =          2       local potential
```

LCOR = T correct aug charges
LPAW = T paw PP
EAUG = 322.069
DEXC = -.001
RMAX = 2.943 core radius for proj-oper
RAUG = 1.300 factor for augmentation sphere
RDEP = 1.993 core radius for depl-charge
QCUT = -4.247; QGAM = 8.494 optimization parameters

Sb:

PAW_GGA Sb 04May1998
5.00000000000000000
parameters from PSCTR are:
VRHFIN =Sb: s2p3
LEXCH = 91
EATOM = 150.2811 eV, 11.0454 Ry
TITEL = PAW_GGA Sb 04May1998
LULTRA = F use ultrasoft PP ?
IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no
RPACOR = 2.200 partial core radius
POMASS = 121.750; ZVAL = 5.000 mass and valenz
RCORE = 2.300 outmost cutoff radius
RWIGS = 2.980; RWIGS = 1.577 wigner-seitz radius (au A)
ENMAX = 172.100; ENMIN = 129.075 eV
ICORE = 3 local potential
LCOR = T correct aug charges
LPAW = T paw PP
EAUG = 380.513
DEXC = -.365
RMAX = 3.515 core radius for proj-oper
RAUG = 1.300 factor for augmentation sphere
RDEP = 2.360 core radius for depl-charge
QCUT = -3.557; QGAM = 7.113 optimization parameters

Te:

PAW_GGA Te 07Sep2001
6.00000000000000000
parameters from PSCTR are:
VRHFIN =Te: s2p4
LEXCH = 91
EATOM = 223.6630 eV, 16.4388 Ry
TITEL = PAW_GGA Te 07Sep2001
LULTRA = F use ultrasoft PP ?
IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

```
RPACOR =    2.200    partial core radius
POMASS =  127.600; ZVAL   =    6.000    mass and valenz
RCORE  =    2.300    outmost cutoff radius
RWIGS  =    2.900; RWIGS  =    1.535    wigner-seitz radius (au A)
ENMAX  =  174.996; ENMIN  =  131.247 eV
ICORE  =        3    local potential
LCOR   =        T    correct aug charges
LPAW   =        T    paw PP
EAUG   =  368.792
DEXC   =    -.121
RMAX   =    3.485    core radius for proj-oper
RAUG   =    1.300    factor for augmentation sphere
RDEP   =    2.397    radius for radial grids
QCUT   =   -3.586; QGAM   =    7.173    optimization parameters
----------------------------------------------------------------------------------------------------
```