Supporting Information

Insight into the inclusion of heteroatom impurities in Silicon structures

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1 Reference systems

1.1 Bulk systems

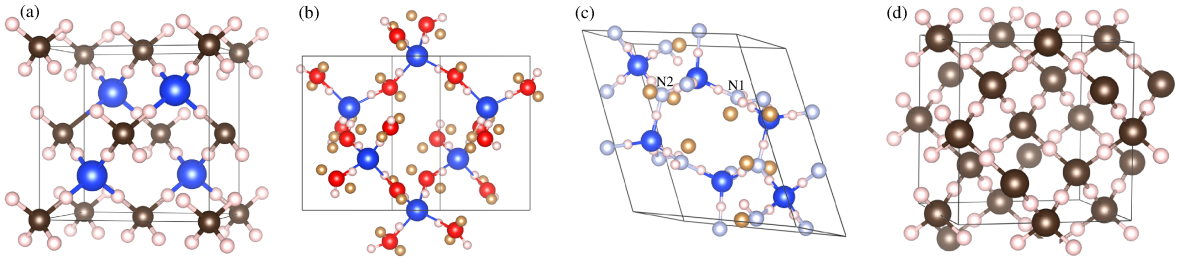

Figure 1: Bonds and lone pairs on (a) SiC (b) SiO_2 (c) Si_3N_4 (d)Diamond

	Si	SiC	SiO_2	Si_3N_4	Diamond
Bond Charges(BC)	1.999	2.000	1.908, 1.957	2.313	1.999
Bond length(BL)Å	2.351	1.896	1.625, 1.628	1.747	1.547
Lone Pair(LP)			4.1340	N2:(0.5289 each) 1.0578	

Table 1: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-C, Si-O, Si-N and C-C bond from respective bilk systems:Si, SiC, SiO_2, Si_3N_4 and diamond.

1.2 Molecular systems

	Ethane	Ethylene	Cyclopropane	Cyclopropene	Bicyclobutane
Bond Charges(BC)	1.81	3.42	1.70	1.80, 3.20	1.87, 1.72
Bond length(BL)Å	1.53	1.33	1.52	1.53, 1.30	1.46, 1.55

Table 2: Bond charge(BC), bond length (BL) of molecular systems

1.3 Silicon grain boundary wthout/with defects

	Bond Charges(BC)	Bond length(BL)Å	LP
Si-GB	2.00329	2.35084	
	2.00096	2.35122	
	1.98795	2.36642	
Si-GB: V1	2.0697	2.32564	Si1: 0.99
	2.0138	2.37601	Si2: 1.00
	2.0138	2.37601	
	2.0192	2.36607	
	2.0192	2.36607	
	2.0712	2.31773	
	2.0712	2.31773	
	1.9712	2.42741	
	2.0282	2.47125	
	2.0062	2.50193	
	2.0280	2.31424	
	2.0280	2.31424	
	1.5429	2.45097	
Si-GB: V2	2.0172	2.37177	Si1: 0.97
	2.0172	2.37177	Si2: 1.03
	2.0609	2.32423	
	2.0609	2.32423	
	2.0676	2.32906	
	2.0676	2.32906	
	1.9926	2.35628	
	1.9782	2.43172	
	2.0207	2.43038	
	2.0207	2.43038	
	2.0273	2.48162	
	2.0251	2.31610	
	1.5522	2.44485	

Table 3: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si bond without/with vacancy defect on Si-GB.

2 Systems with interstitial carbon impurities

2.1 Electronic properties

X	$E_{\mathrm{f}}^{\mathrm{XB}}$	$E_{\mathrm{f}}^{\mathrm{XGB}}$	$E_{\mathrm{f}}^{\mathrm{XV1GB}}$	$E_{\mathrm{f}}^{\mathrm{XV2GB}}$
1C	3.5467	3.5072	-1.6935	-1.8003
2C	4.6315	4.3359	0.4985	0.2165
3C	6.2242	5.2122	0.9758	0.8144
4C	8.1596	7.6275	2.2861	2.1306

Table 4: Formation energy (eV) of Si bulk and $\Sigma 3\{111\}$ Si GB without/with vacancies V1 and V2 with interstitial C atoms from 1 to 4. The values are reported for the lowest energy structures.

X	$E_g^{\text{Si-bulk}}$	E_g^{GB}	E_g^{V1GB}	E_g^{V2GB}
1C	0	0.0477	0.3587	0.4014
2C	0.4291	0.5235	0	0
3C	0.6944	0.4729	0.6066	0.5578
4C	0.4549	0.1319	0.6502	0.5978

Table 5: Energy gaps (eV) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial C atoms from 1 to 4. The values are reported for the lowest energy structures.

X	P(X+B)	P(X+GB)	P(X+V1GB)	P(X+V2GB)
1C	2.564	2.281	0.674	0.673
2C	3.850	2.756	1.507	1.502
3C	3.742	2.845	2.343	2.359
4C	4.734	3.356	2.563	2.543

Table 6: Hydrostatic pressure (GPa) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial C atoms from 1 to 4. The values are reported for the lowest energy structures.

2.2 Bonding analysis

Si-Bulk	BC(Si-Si)	BL(Si-Si)Å	BC(Si-C)	BL(Si-C)Å	BC(C-C)	BL(C-C)Å	LP
1C	1.9917	2.31736	2.4598	1.81289			0.14269
	1.9916	2.31759	2.5371	1.81233			
	1.9950	2.31807	2.3758	1.74694			
	1.9948	2.31842					
	2.2328	2.28068					
	2.2350	2.28173					
	1.9995	2.44675					
2C	1.9779	2.31447	2.4845	1.78563	3.0651	1.31413	
	1.9781	2.31436	2.4843	1.78585			
	1.9779	2.31428	1.7554	1.84197			
	1.9782	2.31450	1.7557	1.84192			
	2.1463	2.25425					
	2.1460	2.25412					
	1.9930	2.30624					
3C	2.0201	2.31590	2.3825	1.81499	1.5792	1.53572	
	2.0046	2.30954	2.3820	1.81535	1.5777	1.53568	
	2.0047	2.30951	1.9941	1.87728	1.41599	1.50008	
	2.0202	2.31584	1.9021	1.87268			
	2.0693	2.34550	1.9028	1.87244			
	2.0693	2.28606					
	2.1675	2.20866					
	1.9581	2.34297					
	1.9577	2.34290					
4C	1.9954	2.36665	2.2361	1.84433	2.1508	1.41648	C3: 0.01604
	2.0178	2.32830	2.3127	1.80898	3.0399	1.34593	
	2.0250	2.38233	2.2938	1.85218	1.7943	1.46732	
	2.0650	2.26366	2.3754	1.81756	1.0551	1.66790	
	2.0407	2.28754	1.9845	1.86359			
	1.9946	2.30892	2.1936	1.87557			
	1.9880	2.31720					
	1.9545	2.34714					
	1.9410	2.35165					

Table 7: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-C and C-C bonds with the inclusion of n numbers of C atoms (n=1,2,3 & 4) in Si-bulk.

Si-GB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-C)	BL(Si-C)Å	BC(C-C)	BL(C-C)Å	LP
1C	1.9903	2.31786	2.2747	1.81425			0.5948
	2.0164	2.31981	2.2497	1.81470			
	1.9814	2.31807	2.4034	1.74762			
	2.2083	2.29283					
	2.0041	2.33252					
	2.2183	2.29363					
	2.0015	2.45067					
2C	2.0507	2.37415	2.3492	1.83840	2.8306	1.37792	
	2.0595	2.36930	2.3430	1.84499			
	2.0793	2.27725	2.1074	1.86866			
	2.0129	2.29788	2.1091	1.86785			
	2.0158	2.29966					
	1.9780	2.34655					
	1.9662	2.35109					
	2.0841	2.26822					
	2.0117	2.34787					
	1.9379	2.31357					
3C	2.0549	2.42702	2.2420	1.85243	1.5274	1.57712	C3: 0.001514
	2.0493	2.30263	2.2603	1.85057			
	2.0167	2.33603	2.2152	1.84016			
	2.0128	2.33161	2.1312	1.85078			
	2.0341	2.35625	2.1595	1.84555			
	2.0395	2.32409	1.8675	1.93941			
	2.0554	2.44381	1.8601	1.93139			
	1.9637	2.32060	1.8795	1.88733			
	2.2222	2.21525	1.6191	1.88109			
			1.5615	1.89062			
4C	2.0053	2.31422	2.3129	1.83722	2.5353	1.39499	
	2.0744	2.32324	2.2215	1.87488			
	2.0044	2.33814	2.1408	1.89536			
	2.0281	2.36433	2.4743	1.78531			
	1.9727	2.34566	2.4729	1.78473			
	1.9471	2.32925	2.4820	1.80381			
	1.8315	2.48968	2.5122	1.77339			
	1.8336	2.44290	2.1517	1.79929			
	1.1289	2.57283	2.7127	1.75854			
			1.7269	1.95371			
			1.1668	2.03012			

Table 8: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-C and C-C bonds with the inclusion of n numbers of C atoms (n=1,2,3 & 4) in Si-GB

	Si-VGB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-C)	BL(Si-C)Å	BC(C-C)	BL(C-C)Å	LP
	1C	2.0243	2.39351	1.9629	1.99583			
		2.0242	2.39361	1.9526	2.00851			
		2.0205	2.39538	1.9201	2.03954			
		2.0289	2.39751	1.9199	2.03983			
		2.0210	2.40463					
		2.0211	2.40463					
		2.0291	2.39740					
		2.0115	2.34935					
		2.0237	2.40396					
		2.0115	2.34945					
		2.0238	2.40392					
		1.9847	2.34152					
		2.0026	2.46212					
		1.9689	2.42414					
V1	2C	2.0236	2.40835	2.4013	1.88745	2.3241	1.41529	
		2.0234	2.42022	2.4174	1.88984			
		2.0299	2.42408	2.4146	1.88913			
		2.0176	2.42635	2.4217	1.88409			
		2.0019	2.33929					
		2.0023	2.34743					
		2.0037	2.34256					
		1.9859	2.37766					
		1.9560	2.37192					
		1.9545	2.37375					
	3C	2.0355	2.32286	2.6560	1.80175	3.0039	1.31195	
		2.0148	2.39841	2.7033	1.80450	1.5660	1.51629	
		2.0329	2.29982	2.1869	1.89111	1.5181	1.52702	
		2.0273	2.33162	2.1780	1.90020			
		2.0332	2.32608					
		1.9774	2.32650					
		1.9799	2.34479					
		1.9779	2.34151					
		2.0099	2.42987					
		1.9848	2.31307					
		1.9863	2.37639					
		1.9979	2.37766					
		1.9875	2.37762					
	4C	2.0668	2.30703	2.3035	1.85418	1.6203	1.53713	C1: 0.010741
		2.0139	2.31936	2.5360	1.83508	1.6193	1.53703	C3: 0.035845
		2.0058	2.34112	2.5114	1.83507	1.5869	1.55733	C3: 0.021072
		2.0131	2.34511	2.3171	1.85991	1.5648	1.55739	
		2.0274	2.37703	2.0619	1.84544	1.3678	1.46903	
		2.0276	2.37684	2.0494	1.90386			
		2.0429	2.35443					
		2.0429	2.35446					
		2.0115	2.29645					
		2.0414	2.36713					

Table 9: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-C and C-C bonds with the inclusion of n numbers of C atoms (n=1,2,3 & 4) in Si-GB with vacancy V1.

	Si-VGB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-C)	BL(Si-C)Å	BC(C-C)	BL(C-C)Å	LP
V2	1C	2.0281	2.38089	1.9623	2.00709			
		2.0281	2.38089	1.9271	2.01777			
		2.0184	2.38908	1.9333	2.03516			
		2.0207	2.40451	1.9333	2.03516			
		2.0207	2.40451					
		2.0272	2.39927					
		2.0272	2.39927					
		2.0224	2.39941					
		2.0224	2.39941					
		2.0196	2.39996					
		2.0022	2.46209					
		2.0022	2.46209					
	2C	2.0119	2.32572	2.3918	1.89263	2.3152	1.41603	
		2.0235	2.40835	2.4065	1.89224			
		2.0171	2.42459	2.4949	1.87145			
		2.0034	2.32550	2.4071	1.88101			
		1.9984	2.38682					
		1.9612	2.35986					
		1.9912	2.33270					
		1.9641	2.41901					
		1.9530	2.37274					
		1.9518	2.37180					
	3C	2.0037	2.33228	2.6418	1.80187	2.9989	1.31248	
		1.9961	2.33392	2.7338	1.79859	1.5669	1.51368	
		1.9890	2.33664	2.1864	1.89848	1.5185	1.52813	
		2.0321	2.30156	2.1773	1.90683			
		2.0308	2.33111					
		2.0230	2.32828					
		2.0121	2.41445					
		2.0278	2.32947					
	4C	2.0689	2.31040	2.2894	1.86170	1.6442	1.53314	
		2.0040	2.33369	2.5498	1.83354	1.6105	1.53866	
		1.9870	2.32764	2.5521	1.84761	1.5948	1.55655	
		2.0023	2.33598	2.3272	1.86247	1.5870	1.55328	
		2.0042	2.33820	2.0410	1.84755	1.3498	1.47835	
		2.0345	2.35649	2.0608	1.90940			
		2.0533	2.31292					
		2.0063	2.33383					
		2.0353	2.34643					

Table 10: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-C and C-C bonds with the inclusion of n numbers of C atoms (n=1,2,3 & 4) in Si-GB with vacancy V2.

3 Systems with interstitial nitrogen impurities

3.1 Electronic properties

X	E_f^{XB}	E_f^{XGB}	E_f^{XV1GB}	E_f^{XV2GB}
1N	1.8155	1.3127	-0.8477	-1.8618
2N	-0.7577	-0.9272	-1.5182	-2.4698
3N	0.5968	-0.4488	-1.8968	-2.0912
4N	1.2163	-1.5700	-3.0445	-4.1177

Table 11: Formation energy (eV) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial N atoms from 1 to 4. The values are reported for the lowest energy structures.

X	$E_g^{Si\text{-}bulk}$	E_g^{GB}	E_g^{V1GB}	E_g^{V2GB}
1N	0	0	0	0
2N	0.5427	0.5444	0.2439	0.6191
3N	0	0	0	0
4N	0.3464	0.6274	0.3966	0.6397

Table 12: Energy gaps (eV) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial N atoms from 1 to 4. The values are reported for the lowest energy structures.

X	P(X+B)	P(X+GB)	P(X+V1GB)	P(X+V2GB)
1N	2.682	2.027	1.601	0.867
2N	2.959	2.577	1.275	0.820
3N	3.161	2.850	1.054	1.327
4N	3.464	3.017	1.331	1.376

Table 13: Hydrostatic pressure (GPa) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial N atoms from 1 to 4. The values are reported for the lowest energy structures.

3.2 Bonding analysis

Si-Bulk	BC(Si-Si)	BL(Si-Si)Å	BC(Si-N)	BL(Si-N)Å	BC(N-N)	BL(N-N)Å	LP
1N	2.0478	2.33613	2.4274	1.66719			2.4509
	1.9314	2.32035	2.4141	1.66703			
	1.9270	2.32165					
	2.0029	2.35253					
	2.0013	2.35318					
	2.0181	2.35985					
	1.9412	2.33676					
	1.9427	2.33660					
2N	2.0849	2.30713	2.2752	1.73464			N1: 1.4121
	2.0843	2.30644	2.2956	1.73455			N2: 1.3700
	2.0843	2.30645	2.0008	1.73999			
	2.0849	2.30701	2.0007	1.73986			
	2.0244	2.31767	2.0293	1.76801			
	2.0239	2.31746	2.0508	1.76801			
3N	2.0352	2.28999	2.2909	1.73687			N1: 0.7259
	2.0792	2.30490	2.3008	1.73777			N2: 0.8651
	2.0869	2.31795	1.9742	1.74611			N3: 1.9743
	2.0827	2.33198	2.0136	1.74460			
	2.0912	2.30624	1.9209	1.76536			
	2.0617	2.28782	2.1595	1.76647			
	2.0273	2.31692	1.8634	1.73632			
	2.0109	2.31369	2.0166	1.76668			
			1.8249	1.78669			
4N	2.0829	2.33553	2.3121	1.73744			N1: 1.2854
	2.0801	2.32301	2.3443	1.71281			N2: 1.3015
	2.0871	2.29693	2.0021	1.75323			N3: 1.5256
	2.1036	2.30566	2.0234	1.74916			N4: 1.9553
	2.1494	2.25315	1.9686	1.75665			
	2.1334	2.35389	1.9389	1.77627			
	1.9851	2.30198	2.2747	1.72530			
			1.9527	1.74615			
			2.0948	1.76061			
			2.0943	1.77118			
			1.9726	1.73255			
			1.7351	1.76306			

Table 14: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-N and N-N bonds with the inclusion of n numbers of N atoms (n=1,2,3 & 4) in Si-bulk.

Si-GB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-N)	BL(Si-N)Å	BC(N-N)	BL(N-N)Å	LP
1N	2.0376	2.32647	2.0010	1.76298			1.9985
	2.0375	2.32636	1.9200	1.74187			
	2.0492	2.32064	1.7552	1.76611			
	2.0493	2.32045					
	2.0331	2.45711					
	2.1035	2.31514					
	2.1035	2.31462					
	2.0271	2.43737					
2N	2.0834	2.31385	2.3180	1.73044			N1: 1.3607
	2.0832	2.31385	2.5108	1.72975			N2: 1.0621
	2.0883	2.31135	2.1484	1.74457			
	2.0881	2.31135	2.0497	1.74220			
	2.0104	2.31162	1.9979	1.77111			
	2.0247	2.32479	1.9923	1.76485			
3N	2.1013	2.29004	2.1939	1.74968			N1: 1.1192
	2.0927	2.31424	2.2970	1.72659			N2: 1.2278
	2.0902	2.30417	2.6832	1.71560			N3: 1.1573
	2.0275	2.32465	2.4427	1.74610			
	2.0207	2.33297	2.2157	1.74352			
	2.0532	2.35819	2.1275	1.73394			
			2.0487	1.71729			
			1.8478	1.75508			
			1.9054	1.79481			
4N	2.1249	2.27680	2.4731	1.73868			N1: 1.4252
	2.0931	2.30091	2.1082	1.76076			N2: 1.0691
	2.0432	2.30684	2.3015	1.72478			N3: 1.1897
	2.0634	2.30310	2.4608	1.72397			N4: 1.2506
	2.0821	2.34419	2.3014	1.74044			
	2.0068	2.31122	2.0111	1.75477			
			2.1785	1.74475			
			2.2933	1.78921			
			1.9397	1.77425			
			2.0967	1.73882			
			1.9236	1.77890			
			1.9361	1.77797			

Table 15: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-N and N-N bonds with the inclusion of n numbers of N atoms (n=1,2,3 & 4) in Si-GB.

	Si-VGB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-N)	BL(Si-N)Å	BC(N-N)	BL(N-N)Å	LP
V1	1N	2.0247	2.41953	2.3100	1.69449			2.9121
		2.0197	2.43623	2.2639	1.69582			
		2.0010	2.35263					
		2.0038	2.34135					
		2.0009	2.35266					
		1.9653	2.38943					
		1.9649	2.38938					
		2.0462	2.30787					
		1.9577	2.38419					
		1.9570	2.38426					
		2.0887	2.32091					
		2.0894	2.31500					
		1.9718	2.30958					
	2N	2.0434	2.34686	1.7099	1.80391	1.0824	1.45049	N1: 2.8568
		2.0256	2.41936	1.6528	1.80577			N2: 3.1440
		2.0453	2.34935	1.5105	1.83934			
		2.0452	2.34960	1.5587	1.83902			
		2.0501	2.33689					
		2.0484	2.35730					
		2.0241	2.44403					
		2.0094	2.34903					
		1.9838	2.33999					
		1.9960	2.55257					
	3N	2.0773	2.41155	2.3000	1.73292			N1: 2.0548
		2.0422	2.37194	1.9799	1.82098			N2: 2.7514
		2.0225	2.33420	1.9268	1.78660			N3: 1.4688
		2.0439	2.40624	2.3839	1.68197			
		1.9813	2.31695	1.9969	1.79269			
		2.0262	2.37227	2.3275	1.70177			
		2.0281	2.42340	1.9324	1.81505			
		2.0372	2.40966	1.7521	1.84096			
		2.0574	2.48591					
	4N	2.1485	2.46424	2.0854	1.74349			N1: 1.8152
		2.0467	2.35171	2.0270	1.73643			N2: 1.2873
		2.0365	2.42135	2.0928	1.77086			N3: 1.2731
		2.0349	2.38921	2.1196	1.75251			N4: 2.2097
		2.0348	2.41911	1.9919	1.77712			
		2.0138	2.36413	2.0611	1.79525			
		1.9812	2.32272	2.0450	1.79535			
		2.0344	2.49119	1.8110	1.76966			
				2.2998	1.80866			
				1.8331	1.84124			
				2.3149	1.77682			
				1.6849	1.80845			

Table 16: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-N and N-N bonds with the inclusion of n numbers of N atoms (n=1,2,3 & 4) in Si-GB with vacancy V1.

	Si-VGB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-N)	BL(Si-N)Å	BC(N-N)	BL(N-N)Å	LP
V2	1N	2.0564	2.36784	1.9553	1.87247			N: 1.6904
		2.0509	2.40413	1.9558	1.87367			Si: 0.4432
		2.0493	2.40528	1.9353	1.86030			
		2.0511	2.38624					
		2.0483	2.38886					
		1.9908	2.40434					
		1.9654	2.40723					
		2.1537	2.33401					
		2.1767	2.33784					
		2.2444	2.32922					
	2N	2.0061	2.31947	2.0590	1.76352			N1: 1.8892
		2.0063	2.31967	2.0490	1.76331			N2: 1.9015
		2.0476	2.36605	1.9409	1.80508			
		2.0227	2.33318	1.9121	1.80526			
		2.0426	2.45558	1.7975	1.82537			
		2.0550	2.53332	1.7913	1.82514			
		2.0549	2.53382					
	3N	2.0252	2.36235	2.4391	1.75975			N1: 1.2519
		2.0156	2.33604	1.9526	1.77458			N2: 2.1413
		2.0422	2.35106	2.7003	1.65230			N3: 2.1548
		2.0451	2.35443	1.9947	1.77620			
		2.0241	2.38609	2.0178	1.78340			
		2.0507	2.43521	2.5160	1.66644			
		2.0473	2.41717	1.8130	1.79287			
		2.0488	2.51035	1.7839	1.81480			
		2.0415	2.51595					
		1.7991	2.35569					
	4N	2.0319	2.28568	2.2734	1.73678			N1: 1.8719
		2.1039	2.42680	2.1041	1.75573			N2: 1.3477
		2.0438	2.26015	2.1349	1.76866			N3: 1.2853
		2.0431	2.35302	2.0410	1.74235			N4: 2.0208
		2.0439	2.35439	2.4054	1.75972			
		2.0269	2.37705	1.9884	1.77301			
		1.9962	2.33643	2.0737	1.76081			
		2.0385	2.42899	1.9729	1.78870			
		2.0439	2.42410	1.8965	1.77478			
		2.0702	2.47255	1.9491	1.77956			
		2.0709	2.51903	1.8610	1.79077			
		2.0000	2.46747	1.7530	1.80498			

Table 17: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si, Si-N and N-N bonds with the inclusion of n numbers of N atoms (n=1,2,3 & 4) in Si-GB with vacancy V2.

4 Systems with interstitial oxygen impurities

4.1 Electronic properties

X	E_f^{XB}	E_f^{XGB}	E_f^{XV1GB}	E_f^{XV2GB}
1O	-2.3649	-2.3950	-4.3281	-4.3036
2O	-5.2126	-5.2515	-7.9224	-7.8855
3O	-8.3195	-8.3974	-11.2368	-11.2213
4O	-11.0994	-11.1843	-14.2579	-14.5924

Table 18: Formation energy (eV) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial O atoms from 1 to 4. The values are reported for the lowest energy structures.

X	$E_g^{Si\text{-}bulk}$	E_g^{GB}	E_g^{V1GB}	E_g^{V2GB}
1O	0.6086	0.5506	0.6274	0.6283
2O	0.5913	0.6073	0.6353	0.6292
3O	0.7285	0.6185	0.6306	0.6319
4O	0.7430	0.5569	0.6850	0.6989

Table 19: Energy gaps (eV) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial O atoms from 1 to 4. The values are reported for the lowest energy structures.

X	P(X+B)	P(X+GB)	P(X+V1GB)	P(X+V2GB)
1O	2.776	2.413	1.697	1.692
2O	3.157	2.660	2.325	2.282
3O	3.479	2.864	2.981	2.616
4O	4.121	3.064	3.171	2.849

Table 20: Hydrostatic pressure (GPa) of Si bulk and Σ3{111} Si GB without/with vacancies V1 and V2 with interstitial O atoms from 1 to 4. The values are reported for the lowest energy structures.

4.2 Bonding analysis

Si-Bulk	BC(Si-Si)	BL(Si-Si)Å	BC(Si-O)	BL(Si-O)Å	LP
1O	1.9918	2.32115	1.7489	1.63550	O1: 4.283
	2.0069	2.32194	1.7479	1.63423	
	2.0467	2.32461			
	2.0555	2.32523			
2O	2.0789	2.30065	1.8939	1.64273	O1: 4.2801
	2.0795	2.30074	1.7391	1.66098	O2: 4.3145
	2.0221	2.32101	1.7493	1.63986	
	1.9685	2.31220	1.5902	1.67594	
	2.0680	2.33876			
	2.0681	2.33886			
	2.0950	2.33589			
3O	2.1373	2.24814	1.9606	1.62698	O1: 4.3299
	1.9904	2.30827	1.9473	1.62684	O2: 4.3404
	2.0606	2.33173	1.9752	1.62684	O3: 4.3299
	2.0602	2.33169	1.5148	1.68729	
	2.0598	2.33175	1.5429	1.68740	
	2.0714	2.35013	1.5191	1.68737	
	2.0710	2.34967			
4O	2.0971	2.22921	1.9675	1.63190	O1: 4.2585
	2.0108	2.32069	1.9450	1.62957	O2: 4.1269
	2.0322	2.32228	1.9281	1.62211	O3: 4.2659
	1.9837	2.30422	1.7651	1.66014	O4: 4.3555
	2.0497	2.33004	1.7301	1.63470	
	2.0734	2.34109	1.7331	1.65317	
			1.6537	1.66647	
			1.5824	1.68762	

Table 21: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si and Si-O bonds with the inclusion of n numbers of O atoms (n=1,2,3 & 4) in Si-bulk.

Si-GB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-O)	BL(Si-O)Å	LP
1O	2.0093	2.32532	1.7792	1.63913	4.2934
	1.9902	2.32383	1.7035	1.63789	
	2.0134	2.33911			
	2.0425	2.32990			
	2.0564	2.32704			
	2.0781	2.32612			
	1.9997	2.32640			
	1.9931	2.34696			
	1.9959	2.36746			
2O	2.0872	2.31206	1.9142	1.64514	O1: 4.3003
	2.0250	2.32108	1.7951	1.64091	O2: 4.3380
	2.0197	2.32159	1.7078	1.66111	
	2.0920	2.31034	1.5149	1.67498	
	2.0950	2.33289			
	2.0132	2.35452			
	2.0226	2.32704			
	1.9877	2.36383			
	1.9847	2.32704			
	1.9957	2.35741			
3O	2.1448	2.25427	1.9600	1.62934	O1: 4.2309
	2.1231	2.28737	2.0395	1.62583	O2: 4.3284
	2.0699	2.34079	1.9255	1.63628	O3: 4.3491
	2.0687	2.36253	1.5670	1.68212	
	2.0445	2.33292	1.5497	1.68240	
	2.0624	2.34653	1.5057	1.69960	
	1.9502	2.32814			
	1.9914	2.33156			
	1.9873	2.33906			
4O	1.9968	2.30698	2.1162	1.60775	O1: 4.1798
	2.0109	2.31411	1.9557	1.60825	O2: 4.3162
	2.0089	2.29839	2.0040	1.60321	O3: 4.4751
	2.0324	2.32370	1.9907	1.61242	O4: 4.3444
	2.0459	2.36708	1.5109	1.69476	
	2.0352	2.32384	1.5546	1.69474	
	2.0739	2.37431	1.5502	1.69645	
	2.1489	2.29031	1.4290	1.71093	
	1.9766	2.33417			

Table 22: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si and Si-O bonds with the inclusion of n numbers of O atoms (n=1,2,3 & 4) in Si-GB

	Si-VGB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-O)	BL(Si-O)Å	LP
V1	1O	2.0433	2.35933	1.5763	1.70276	4.8177
		2.0432	2.35930	1.4038	1.70352	
		2.0504	2.34937			
		2.0503	2.34933			
		2.0493	2.41995			
		2.0374	2.44706			
		2.0781	2.32314			
		2.0788	2.31593			
		2.0029	2.31171			
	2O	2.0854	2.34609	1.8687	1.63189	O1: 4.5218
		2.0853	2.34610	1.6492	1.68177	O2: 4.2086
		1.9984	2.31011	1.7409	1.66199	
		2.0531	2.38759	1.6583	1.66506	
		2.0612	2.35561			
		2.0613	2.35561			
		2.0745	2.32627			
		2.0759	2.32289			
		2.0046	2.31500			
		1.5825	2.45085			
	3O	2.0851	2.31788	1.8948	1.62656	O1: 4.2695
		2.0886	2.32236	1.8150	1.63978	O2: 4.1855
		2.0016	2.31408	1.7386	1.62749	O3: 4.3248
		2.0592	2.34710	1.7672	1.63987	
		2.0592	2.34711	1.7558	1.65652	
		2.0446	2.31293	1.7408	1.65403	
		2.0107	2.32353			
		1.9913	2.34144			
		1.9769	2.33572			
		2.0050	2.31155			
	4O	2.1503	2.27352	2.0133	1.62843	O1: 4.1015
		2.0809	2.31442	1.8618	1.62652	O2: 4.1822
		2.0001	2.31435	1.8409	1.64666	O3: 4.2785
		1.9944	2.30186	1.7146	1.66121	O4: 4.2594
		2.0569	2.32987	1.9526	1.62095	
		2.0262	2.30338	1.8908	1.62452	
		2.0582	2.34486	1.7483	1.65339	
		2.0608	2.34711	1.5363	1.69373	
		2.0576	2.38358			
		2.0007	2.33742			
		1.9774	2.34089			

Table 23: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si and Si-O bonds with the inclusion of n numbers of O atoms (n=1,2,3 & 4) in Si-GB with vacancy V1.

	Si-VGB	BC(Si-Si)	BL(Si-Si)Å	BC(Si-O)	BL(Si-O)Å	LP
V2	1O	2.0490	2.35202	1.5907	1.70536	4.7927
		2.0490	2.35202	1.4133	1.70324	
		2.0389	2.34423			
		2.0479	2.39899			
		2.0479	2.39899			
		2.0459	2.42851			
		2.0673	2.32292			
		2.0017	2.31335			
		1.5752	2.43705			
	2O	2.0916	2.34935	1.7851	1.63329	O1: 4.3862
		2.0916	2.34935	1.6953	1.66673	O2: 4.3375
		2.0257	2.32115	1.7470	1.68194	
		2.0257	2.32115	1.6959	1.66639	
		2.0504	2.36999			
		2.0504	2.36999			
		2.0360	2.33241			
		2.0735	2.37747			
		2.0611	2.32703			
		2.0018	2.31163			
		1.6003	2.43229			
	3O	2.0823	2.30486	1.8844	1.65237	O1: 4.4063
		2.0826	2.30432	1.7179	1.64360	O2: 4.2758
		2.0494	2.35862	1.6933	1.64503	O3: 4.3626
		2.0494	2.35862	1.7372	1.66772	
		2.0304	2.32693	1.7276	1.66736	
		2.0309	2.32429	1.6871	1.65621	
		2.0363	2.30348			
		1.9855	2.32768			
		2.0048	2.31078			
		1.5979	2.42764			
	4O	2.1604	2.33661	1.8891	1.63356	O1: 4.2751
		2.0939	2.32015	1.9768	1.61832	O2: 4.1492
		2.0371	2.34213	1.8987	1.64051	O3: 4.3613
		2.0210	2.31449	1.8329	1.66554	O4: 4.1261
		2.0529	2.36183	1.7697	1.64925	
		2.0454	2.35171	1.7404	1.65316	
		2.0487	2.34450	1.6899	1.67462	
		2.0529	2.32527	1.6799	1.67034	
		2.0686	2.32756			
		2.0095	2.32386			
		1.6214	2.41121			

Table 24: Bond charge(BC), bond length (BL) and lone pair(LP) data for Si-Si and Si-O bonds for the inclusion of n numbers of O atoms (n=1,2,3 & 4) in Si-GB with vacancy V2.

5 Bond charge variations

5.1 Nitrogen

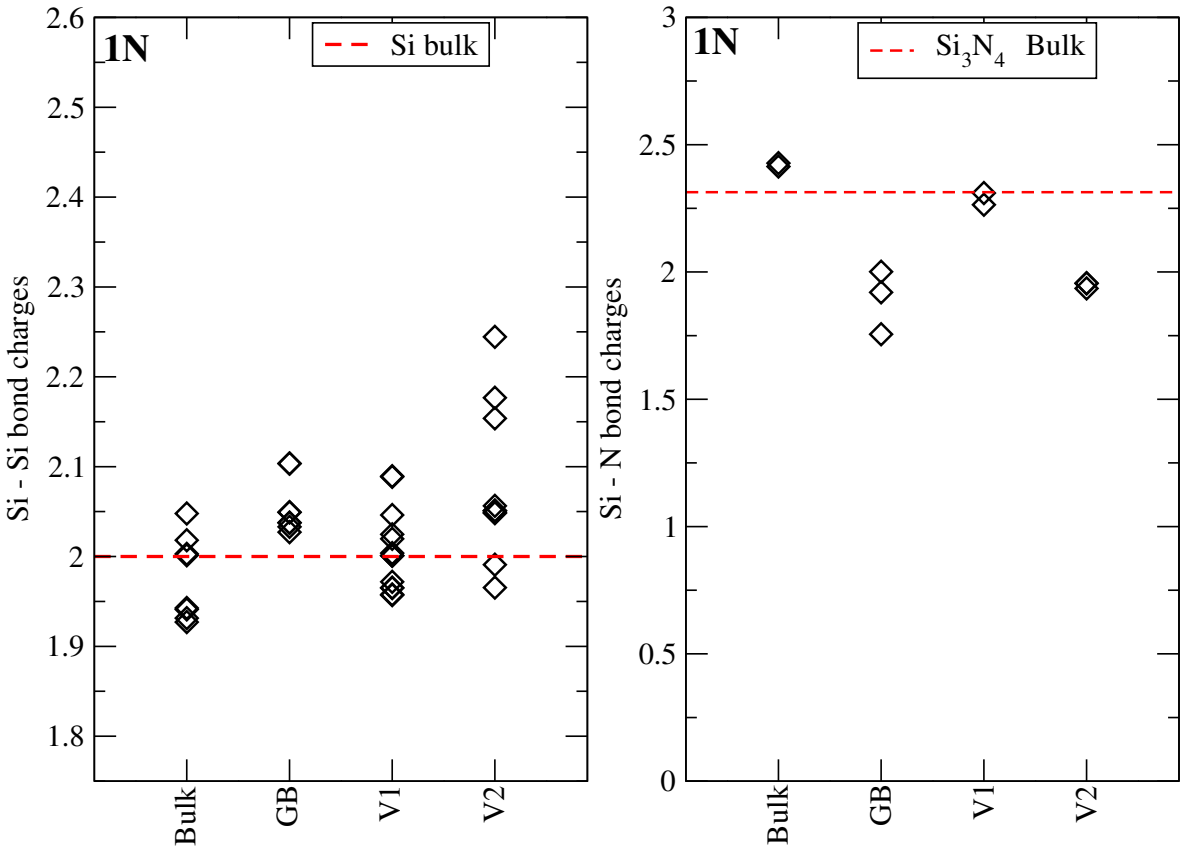

Figure 2: Bond charge variation of Si-Si and Si-N with the inclusion of one nitrogen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond charges from bulk phases of Si and Si_3N_4 are marked in the inset of respective plots.

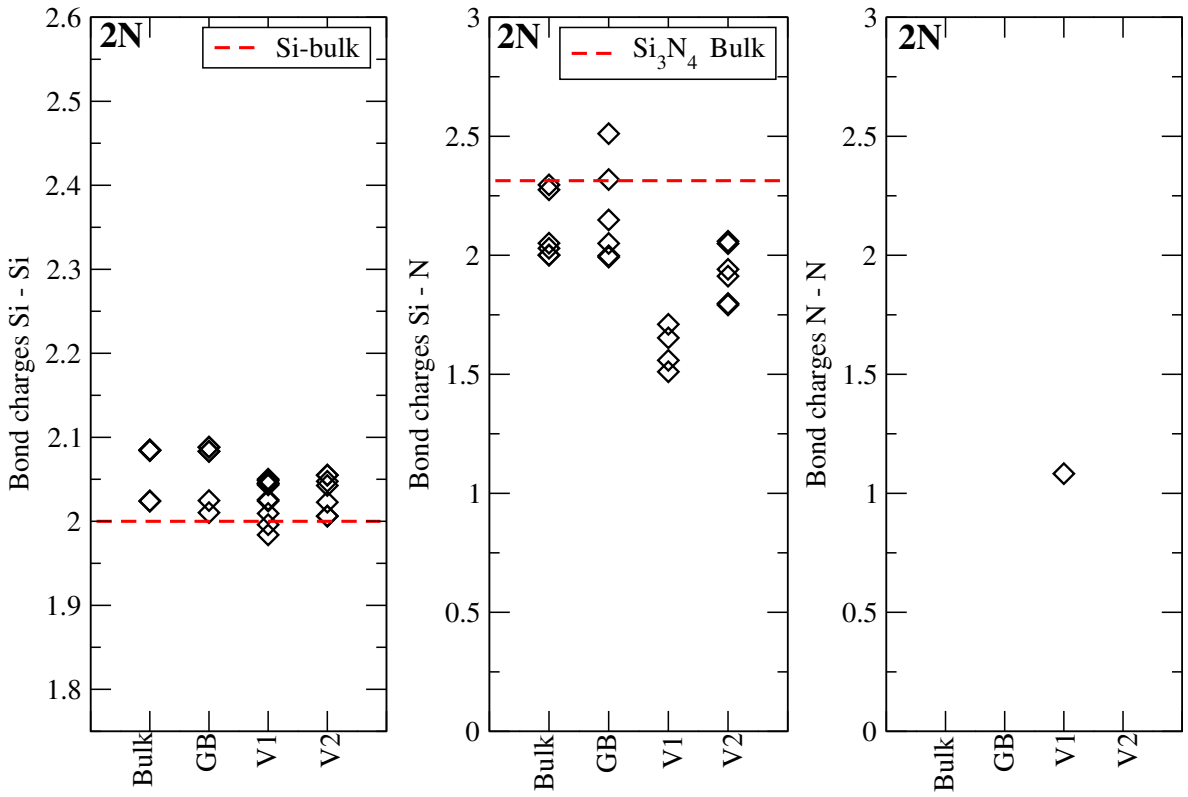

Figure 3: Bond charge variation of Si-Si, Si-N and N-N for the inclusion of two nitrogen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond charges from bulk phases of Si and Si_3N_4 are marked in the inset of respective plots.

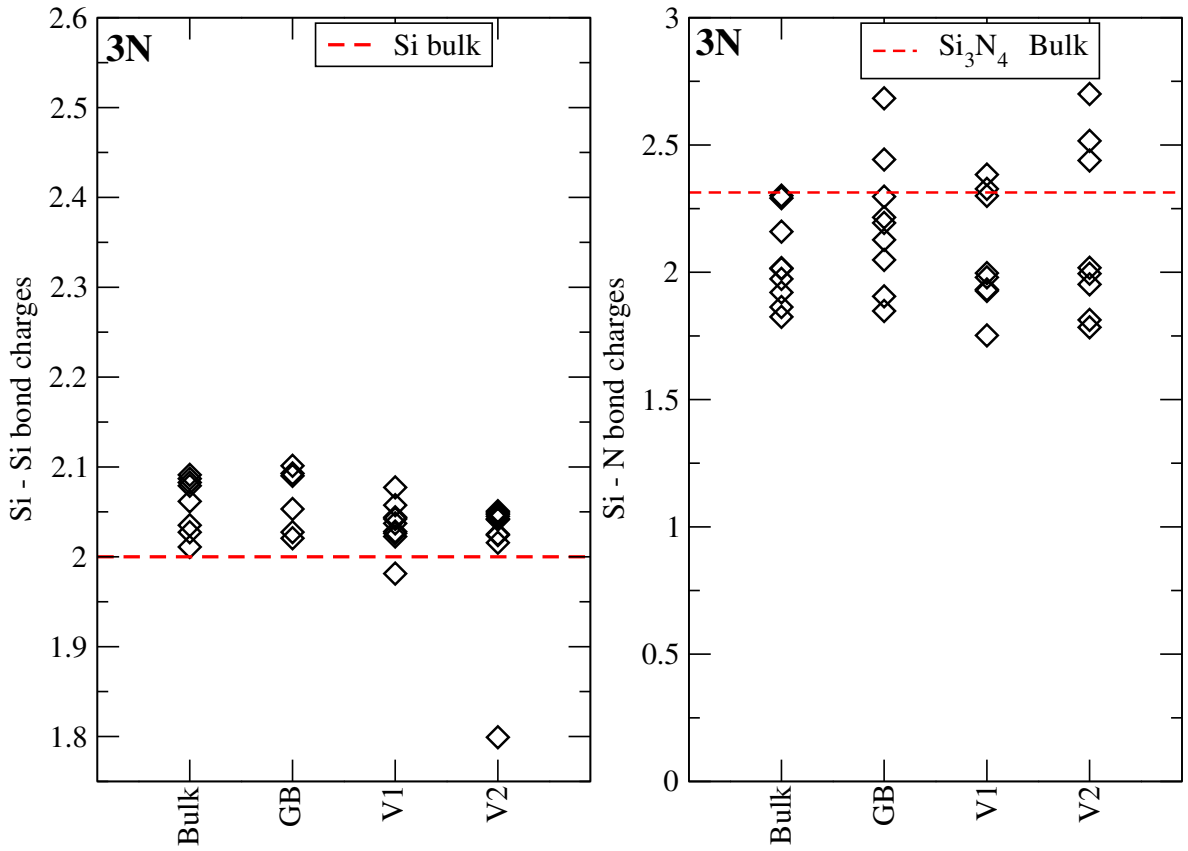

Figure 4: Bond charge variation of Si-Si and Si-N for the inclusion of three nitrogen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond charges from bulk phases of Si and Si_3N_4 are marked in the inset of respective plots.

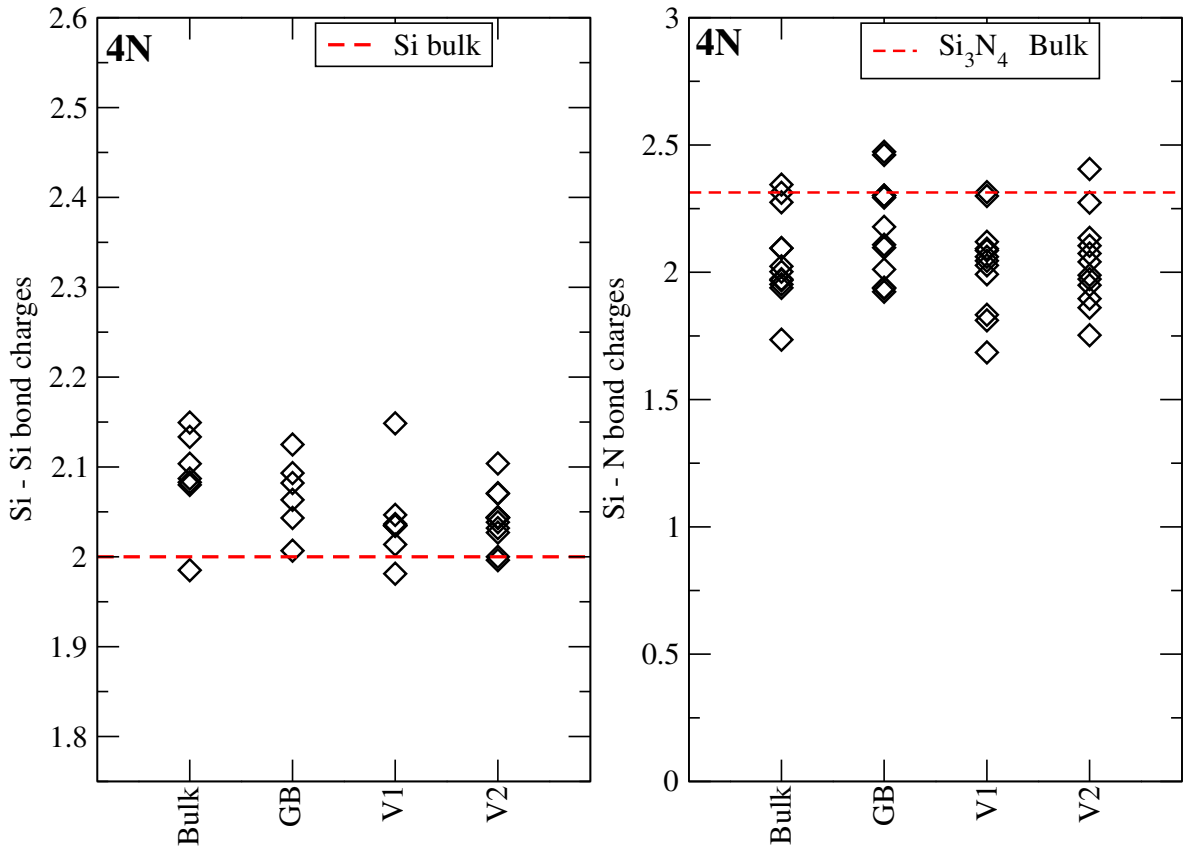

Figure 5: Bond charge variation of Si-Si and Si-N for the inclusion of four nitrogen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond charges from bulk phases of Si and Si_3N_4 are marked in the inset of respective plots.

5.2 Oxygen

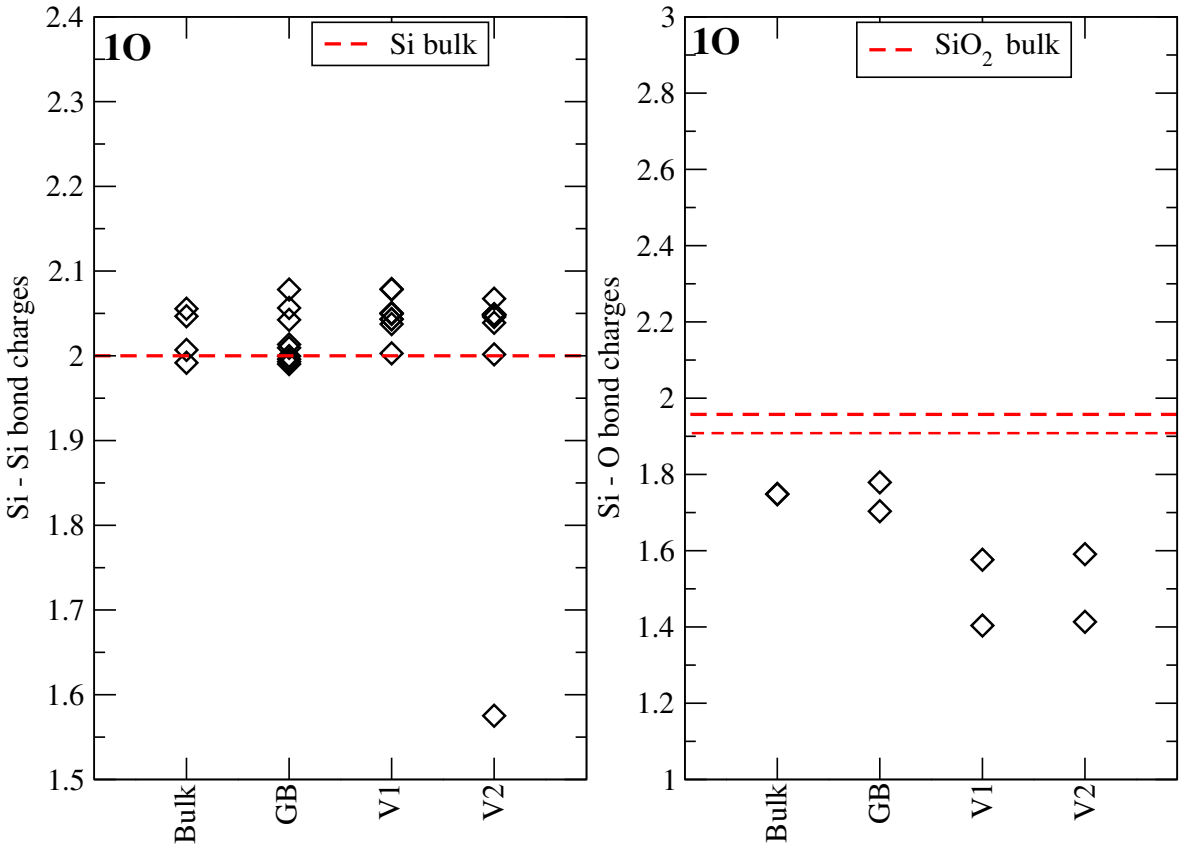

Figure 6: Bond charge variation of Si-Si and Si-O for the inclusion of one oxygen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond charges from bulk phases of Si and SiO_2 are marked in the inset of respective plots.

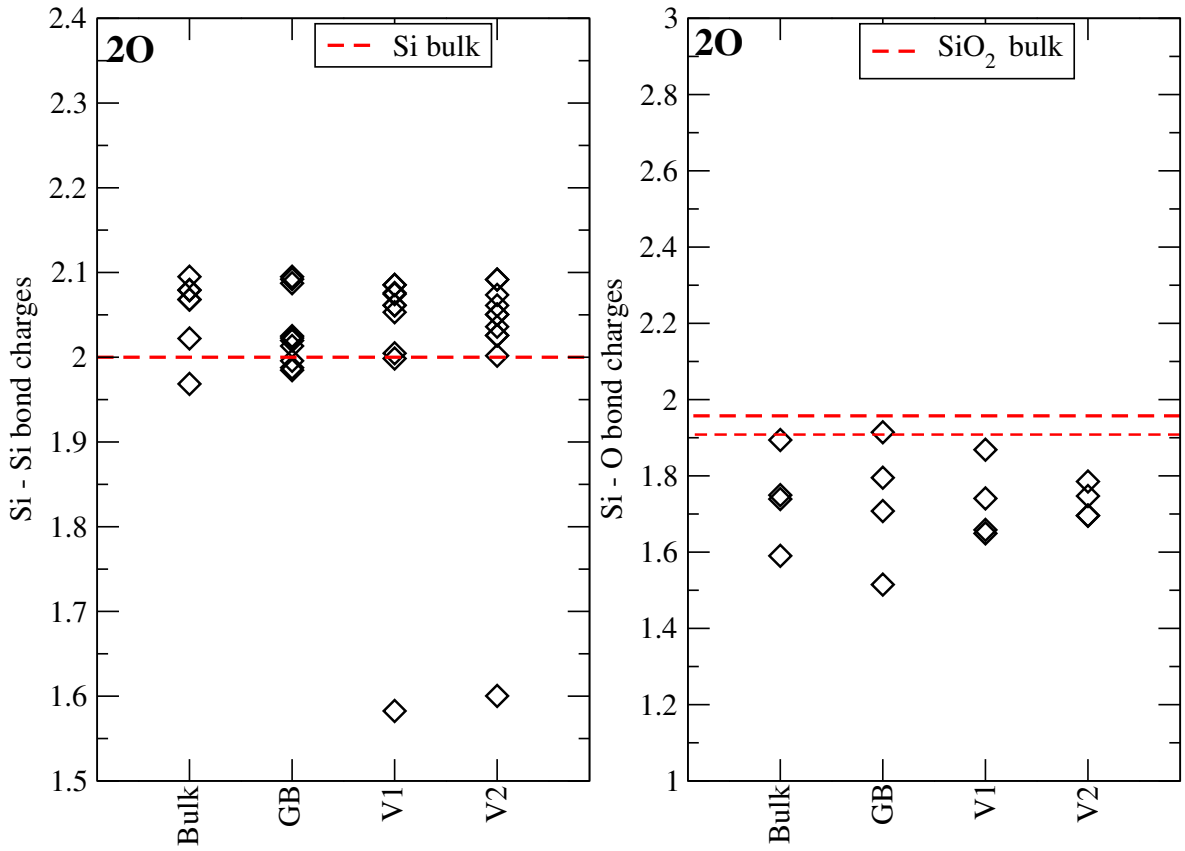

Figure 7: Bond charge variation of Si-Si and Si-O for the inclusion of two oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond charges from bulk phases of Si and SiO_2 are marked in the inset of respective plots.

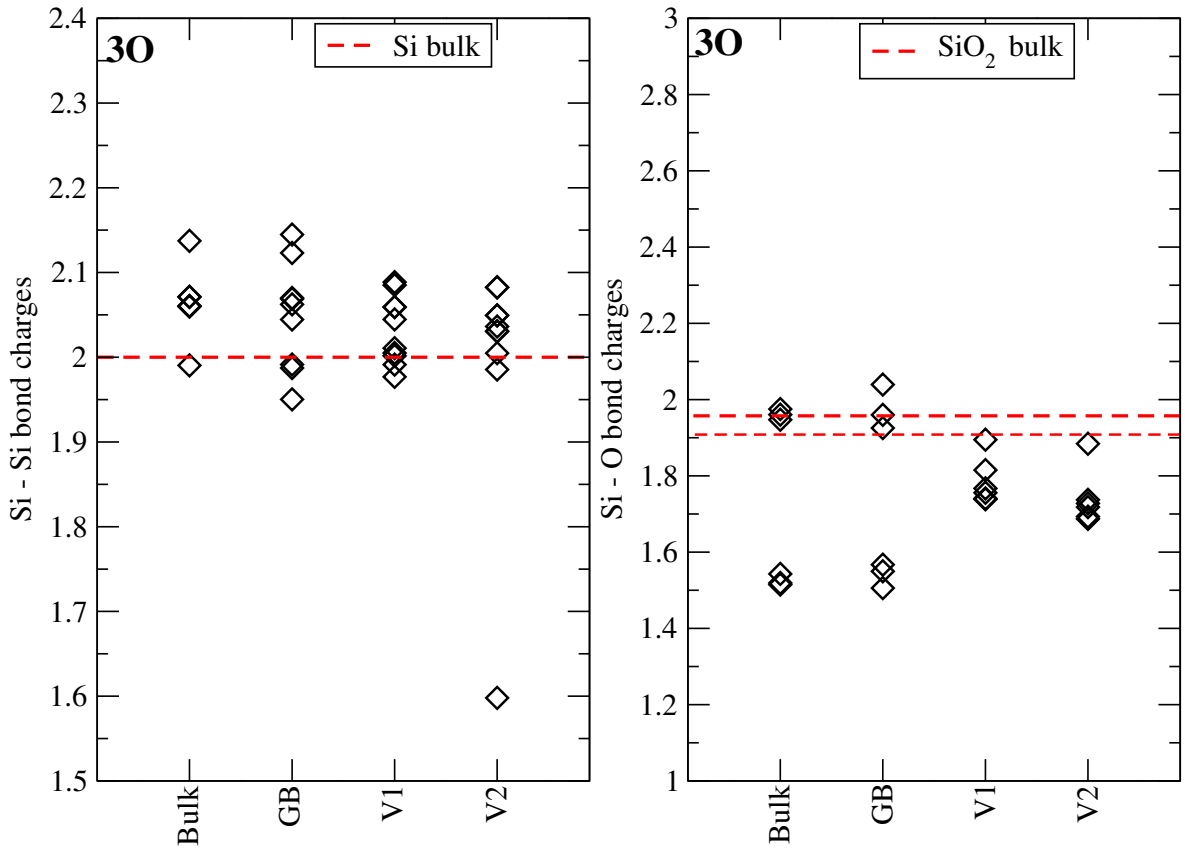

Figure 8: Bond charge variation of Si-Si and Si-O for the inclusion of three oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond charges from bulk phases of Si and SiO_2 are marked in the inset of respective plots.

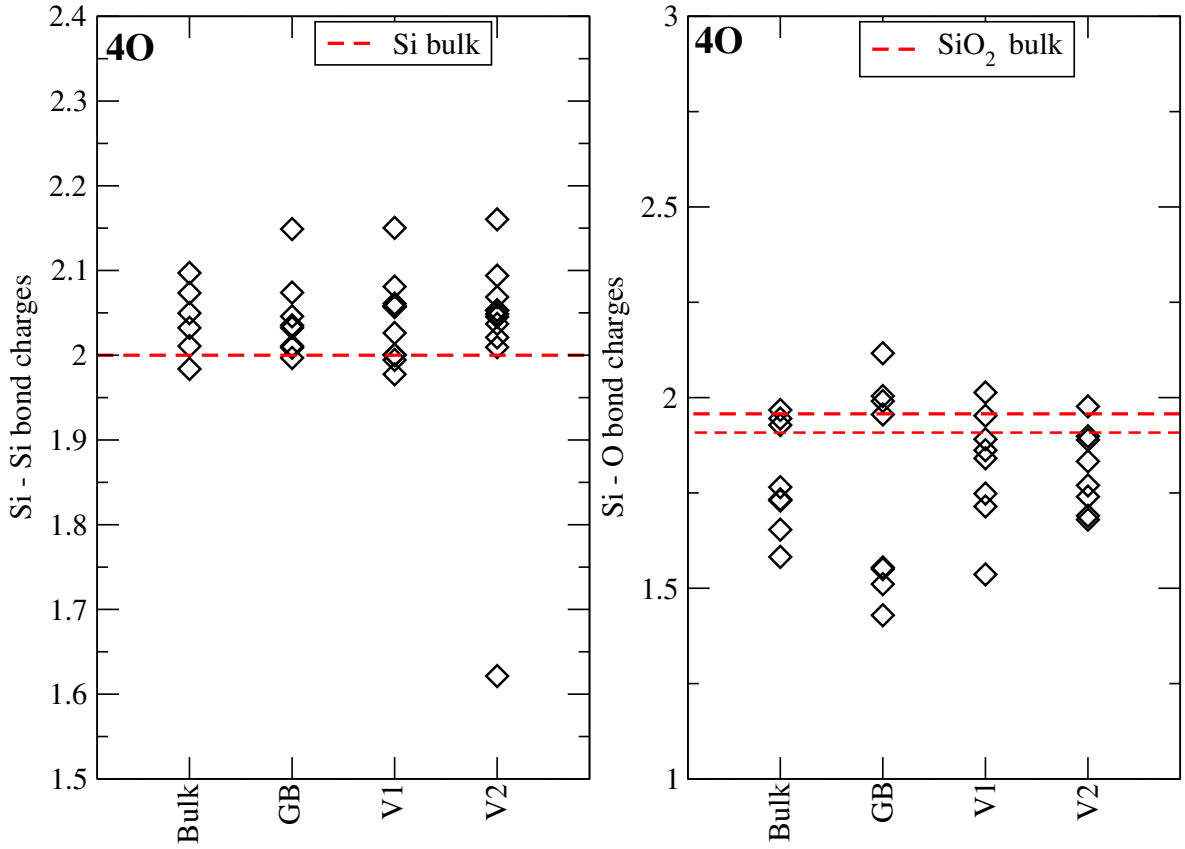

Figure 9: Bond charge variation of Si-Si and Si-O for the inclusion of four oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond charges from bulk phases of Si and SiO_2 are marked in the inset of respective plots.

6 Bond length variations

6.1 Carbon

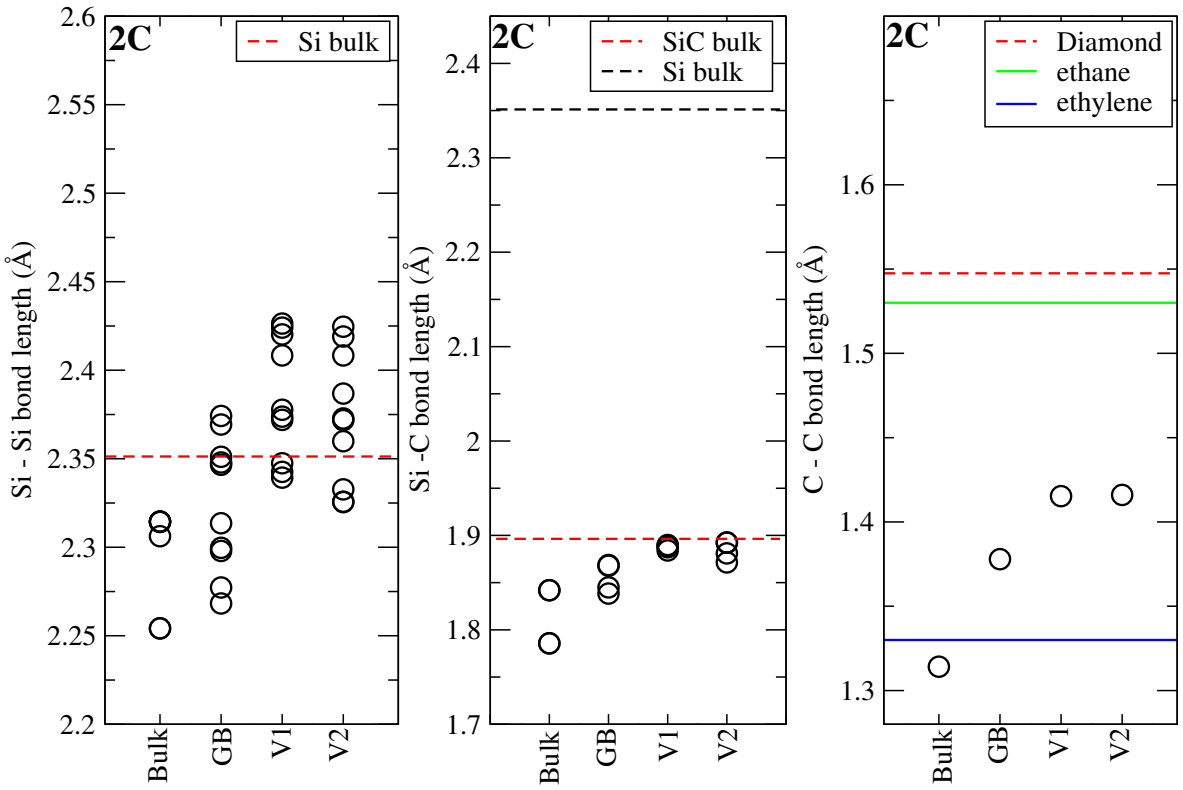

Figure 10: Bond length variation of Si-Si, Si-C and C-C for the inclusion of two carbon atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-C/C-C bond length from bulk phases of Si, SiC, diamond and molecular systems ethylene and ethane are marked in the inset of respective plots.

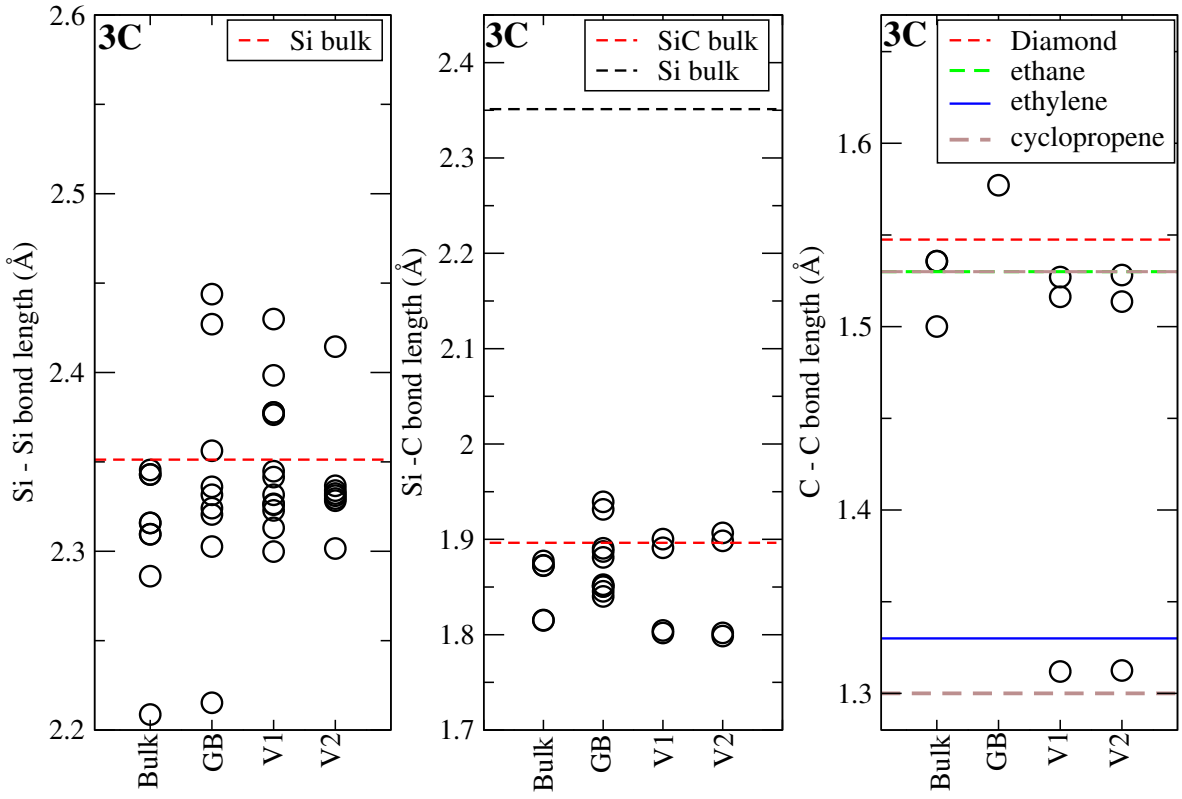

Figure 11: Bond length variation of Si-Si, Si-C and C-C for the inclusion of three carbon atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-C/C-C bond length from bulk phases of Si, SiC, diamond and molecular systems ethylene, ethane, and cyclopropen are marked in the inset of respective plots

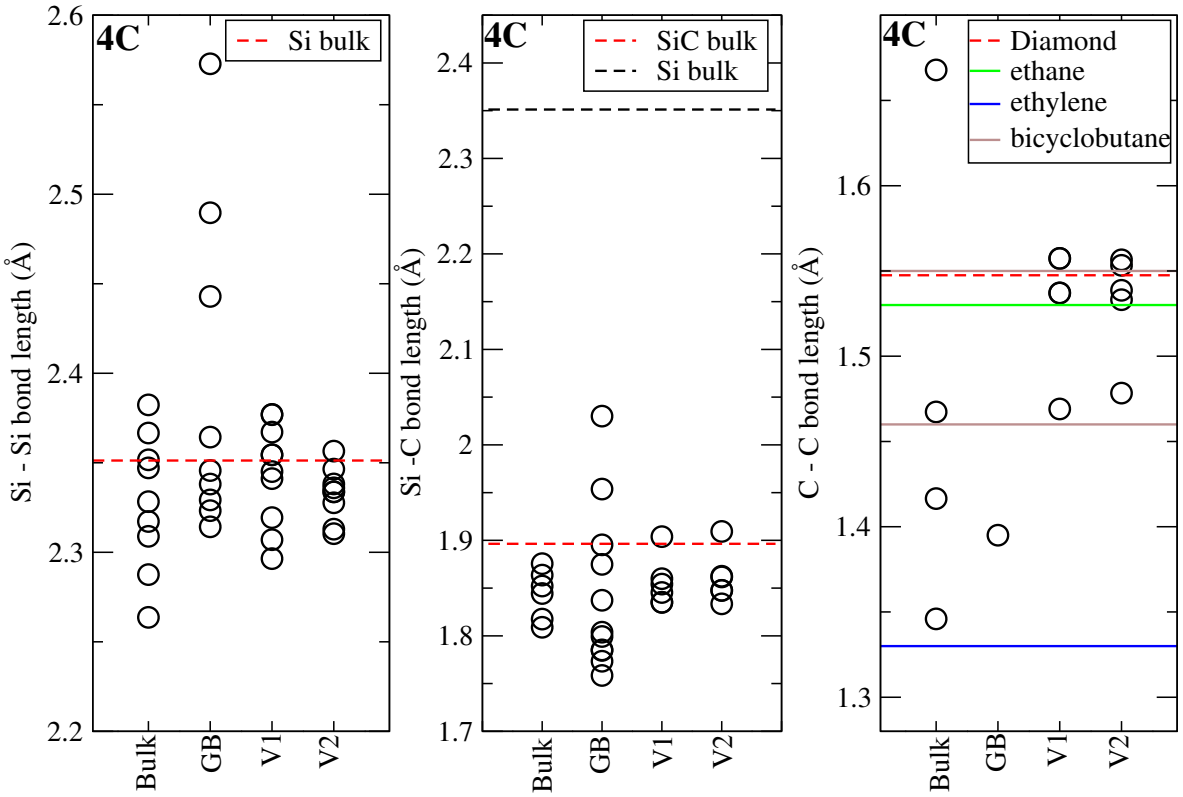

Figure 12: Bond length variation of Si-Si, Si-C and C-C for the inclusion of four carbon atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-C/C-C bond length from bulk phases of Si, SiC, diamond and molecular systems ethylene, ethane, and bicyclobutane are marked in the inset of respective plots

6.2 Nitrongen

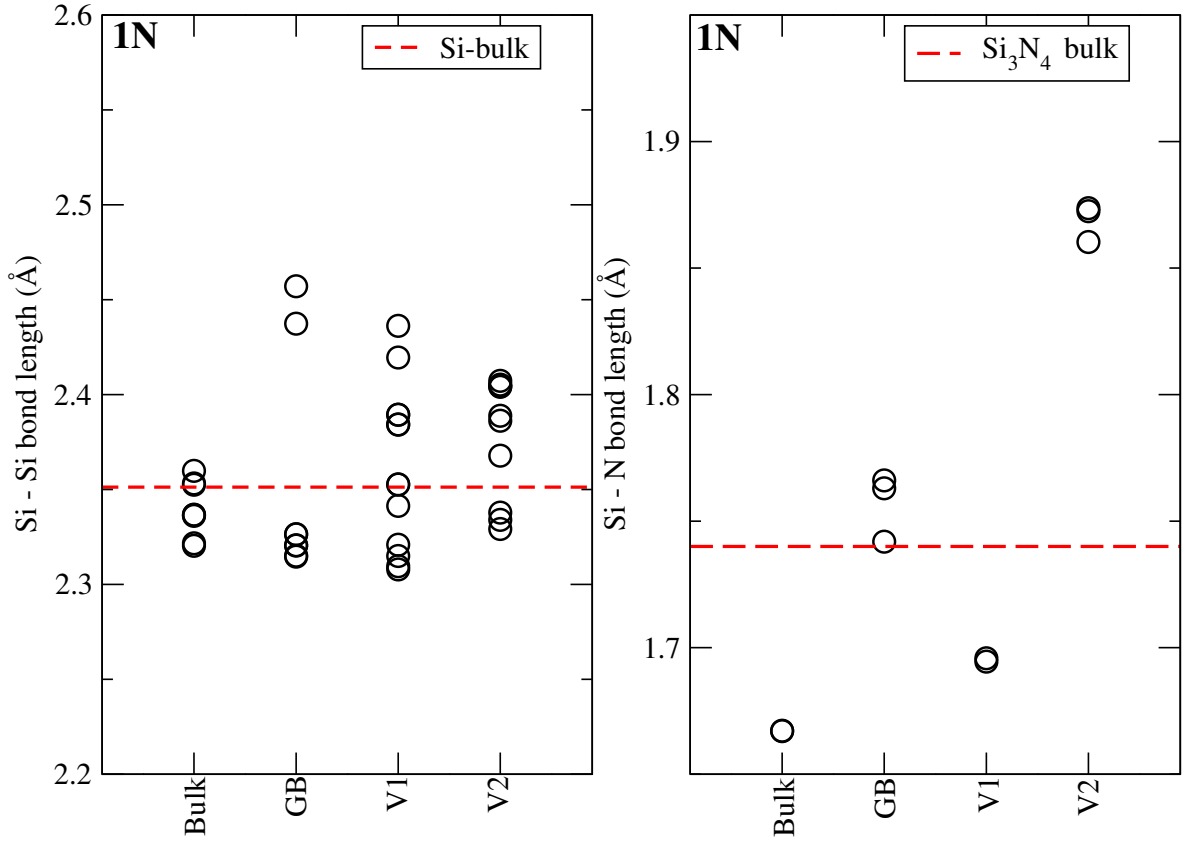

Figure 13: Bond length variation of Si-Si and Si-N for the inclusion of one nitrogen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond length from bulk phases of Si, Si_3N_4 are marked in the inset of respective plots.

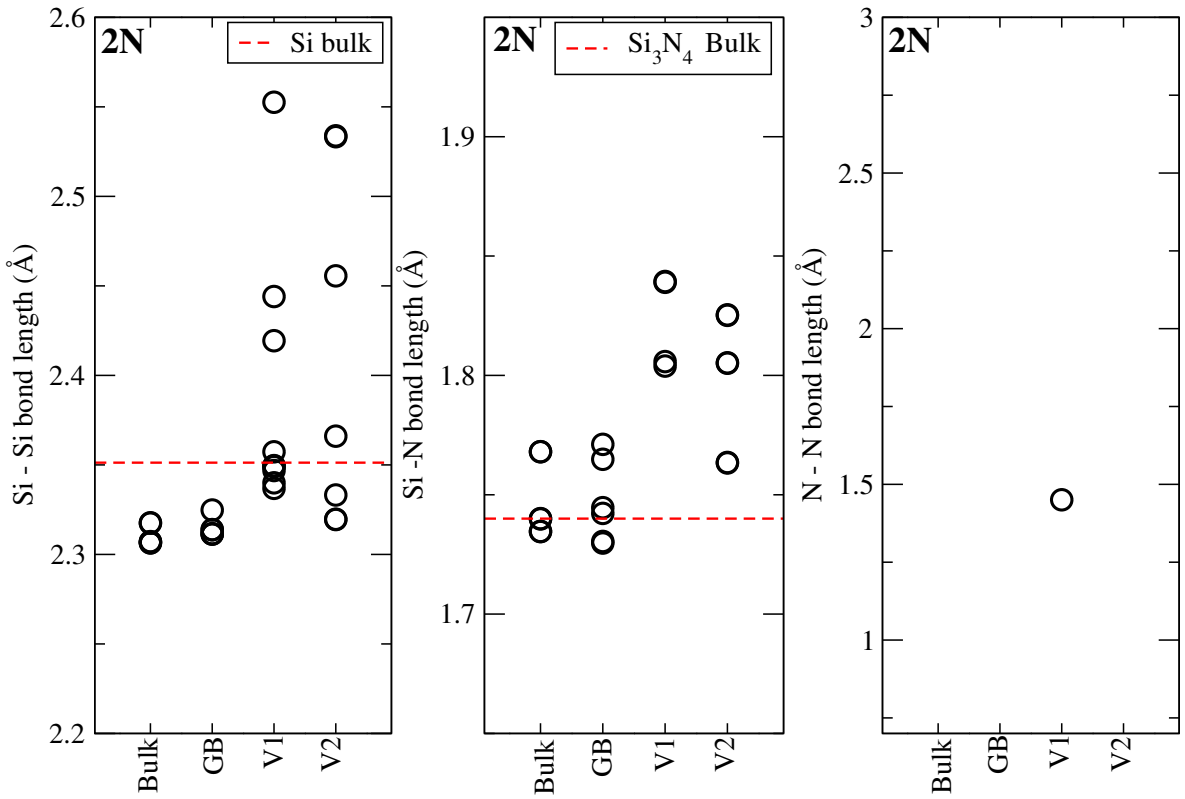

Figure 14: Bond length variation of Si-Si, Si-N and N-N for the inclusion of two nitrogen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond length from bulk phases of Si, Si_3N_4 are marked in the inset of respective plots.

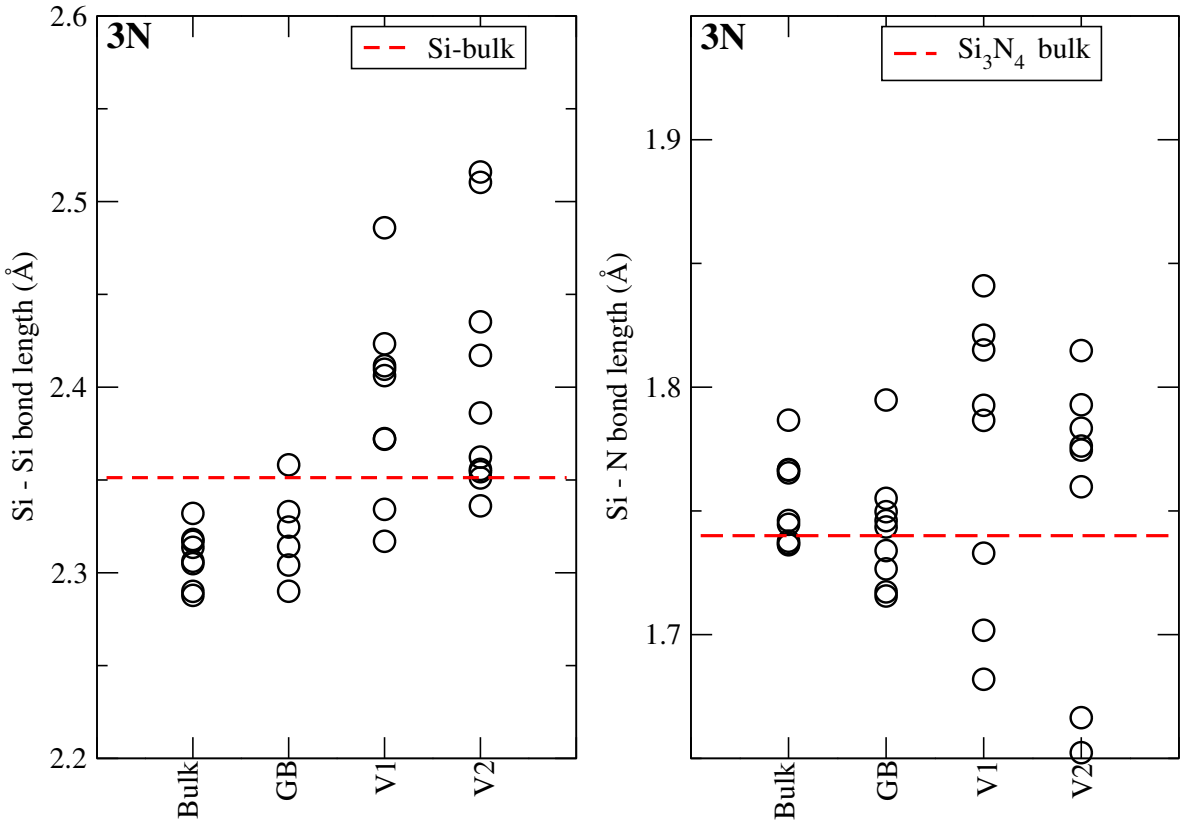

Figure 15: Bond length variation of Si-Si and Si-N for the inclusion of three nitrogen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond length from bulk phases of Si, Si_3N_4 are marked in the inset of respective plots.

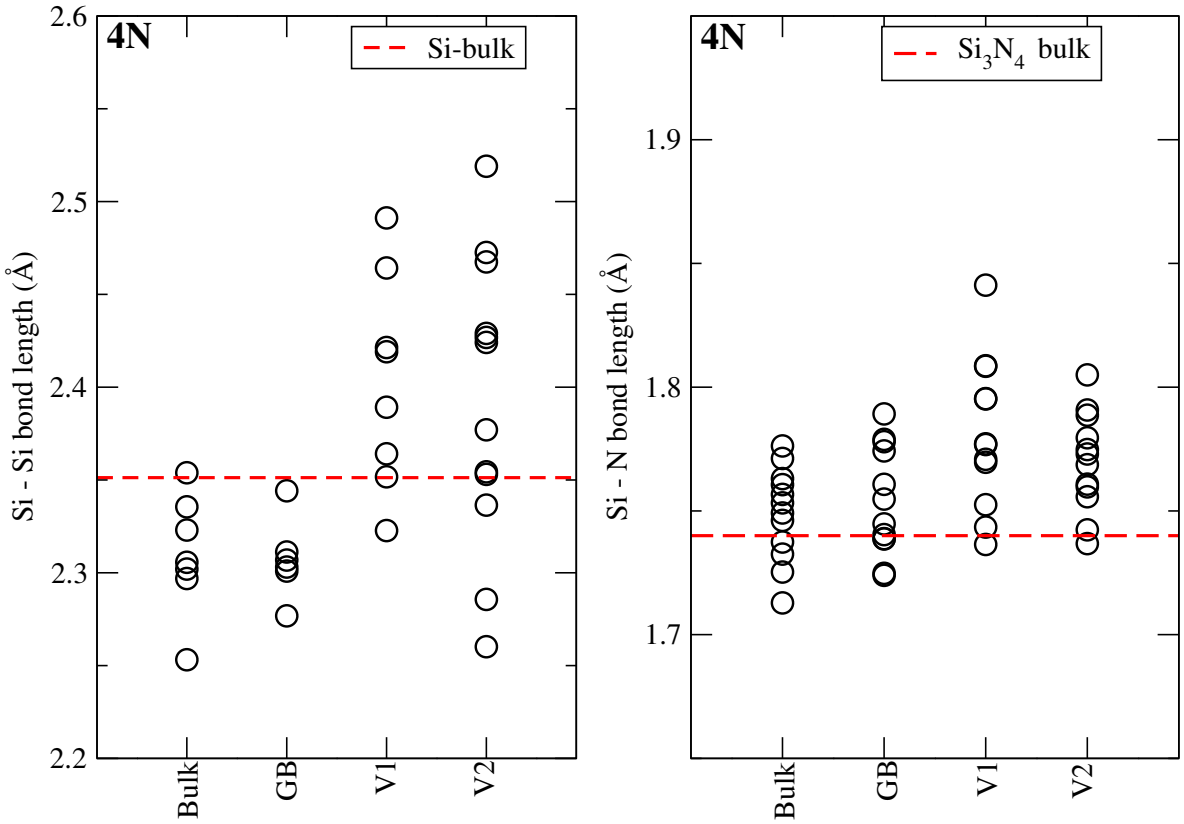

Figure 16: Bond length variation of Si-Si and Si-N for the inclusion of four nitrogen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-N bond length from bulk phases of Si, Si_3N_4 are marked in the inset of respective plots.

6.3 Oxygen

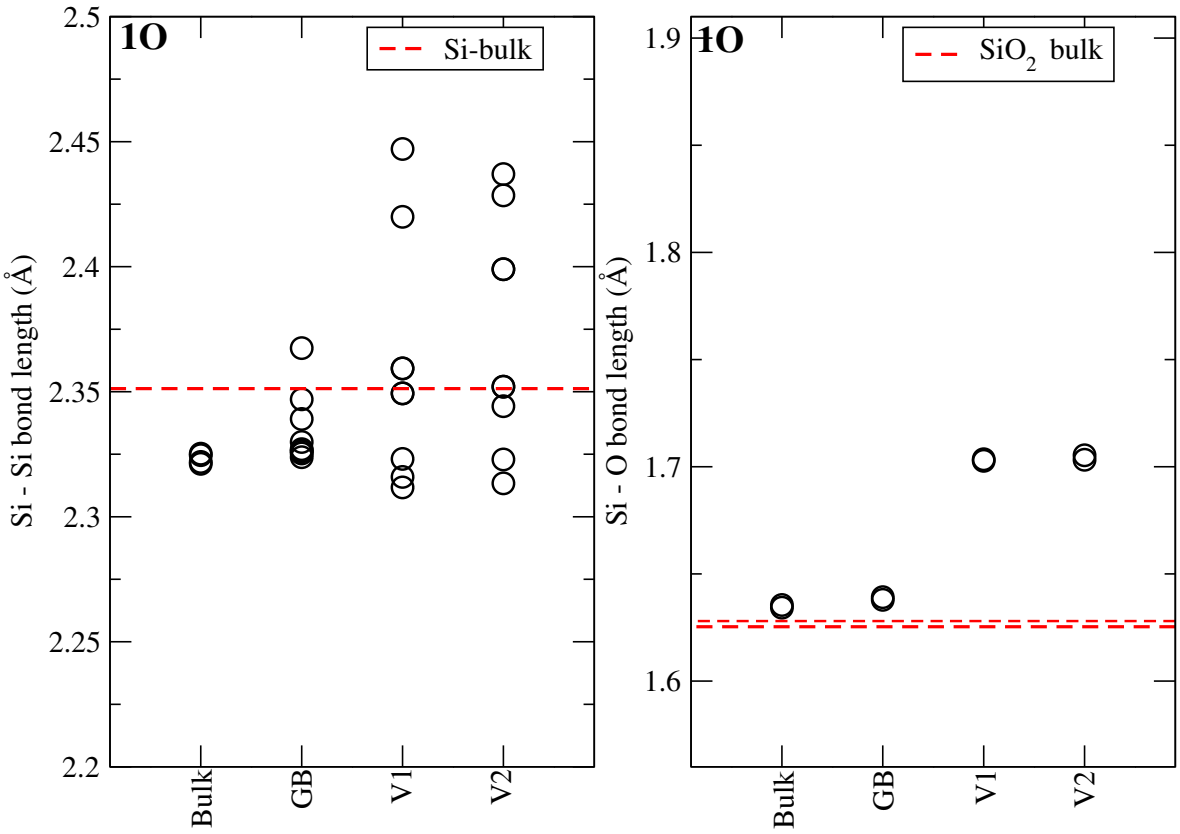

Figure 17: Bond length variation of Si-Si and Si-O for the inclusion of one oxygen atom in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond length from bulk phases of Si, SiO_2 are marked in the inset of respective plots.

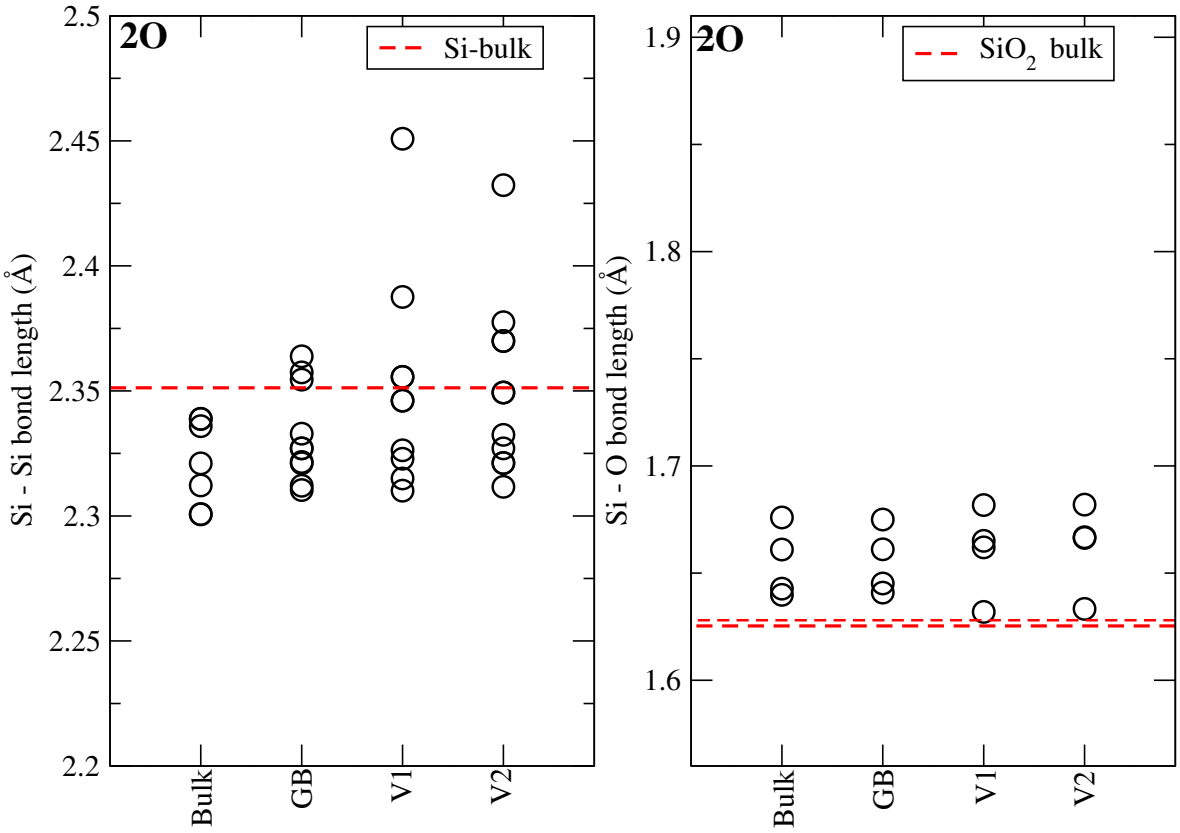

Figure 18: Bond length variation of Si-Si and Si-O for the inclusion of two oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond length from bulk phases of Si, SiO_2 are marked in the inset of respective plots.

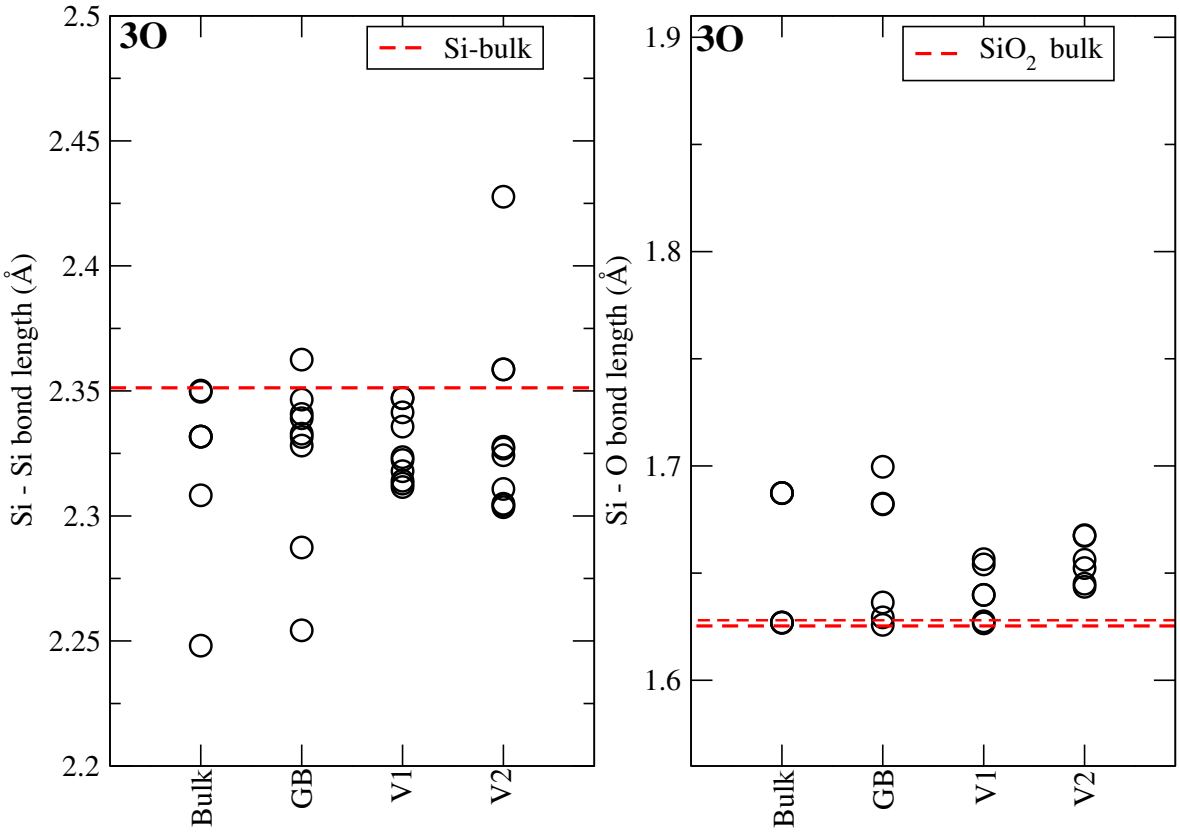

Figure 19: Bond length variation of Si-Si and Si-O for the inclusion of three oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond length from bulk phases of Si, SiO_2 are marked in the inset of respective plots.

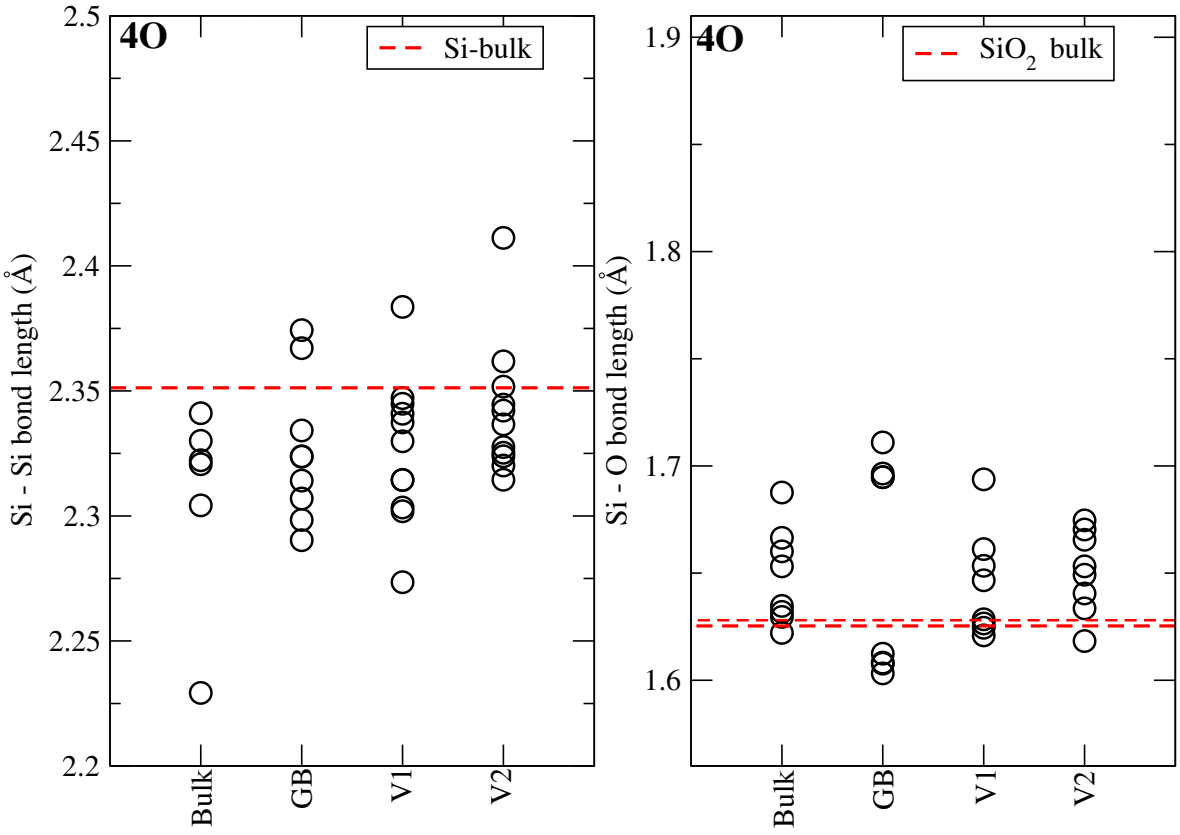

Figure 20: Bond length variation of Si-Si and Si-O for the inclusion of four oxygen atoms in Si-bulk, Si-GB and in presence of vacancy V1 and V2. As a reference, Si-Si/Si-O bond length from bulk phases of Si, SiO_2 are marked in the inset of respective plots.