Supporting information for

Diffusion of lithium in bulk amorphous silicon: a theoretical study

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Model amorphous silicon unit cell

Lattice vectors

a (11.096, -0.172, 0.189)
b (-0.172, 11.217 , -0.077)
C (0.189, -0.077, 11.109)

Scaled atom positions (a, b, c)

a	b	c	a	b	c
0.355	0.923	0.794	0.191	0.374	0.012
0.339	0.643	0.338	0.043	0.528	0.031
0.289	0.724	0.853	0.456	0.297	0.718
0.640	0.593	0.199	0.171	0.501	0.368
0.460	0.489	0.262	0.035	0.860	0.032
0.730	0.917	0.252	0.057	0.900	0.352
0.547	0.247	0.512	0.525	0.971	0.283
0.816	0.461	0.594	0.846	0.369	0.252
0.537	0.723	0.069	0.829	0.047	0.654
0.580	0.185	0.849	0.214	0.295	0.355
0.735	0.727	0.345	0.101	0.328	0.686
0.564	0.965	0.817	0.946	0.706	0.373
0.275	0.085	0.106	0.896	0.036	0.318
0.790	0.187	0.812	0.485	0.505	0.748
0.824	0.917	0.058	0.513	0.036	0.492
0.254	0.082	0.894	0.386	0.807	0.204
0.433	0.597	0.937	0.666	0.589	0.669
0.388	0.435	0.066	0.648	0.939	0.618
0.673	0.828	0.939	0.430	0.291	0.342
0.257	0.282	0.821	0.149	0.512	0.583
0.338	0.933	0.578	0.144	0.234	0.164
0.317	0.615	0.672	0.884	0.110	0.984
0.136	0.984	0.536	0.192	0.900	0.177
0.898	0.366	0.764	0.936	0.191	0.176
0.889	0.162	0.486	0.998	0.536	0.249
0.622	0.743	0.533	0.404	0.737	0.520
0.053	0.018	0.894	0.968	0.616	0.567

0.756	0.317	0.447	0.957	0.734	0.745
0.547	0.288	0.038	0.466	0.149	0.184
0.086	0.697	0.910	0.100	0.196	0.515
0.000	0.938	0.703	0.772	0.669	0.836
0.718	0.423	0.093	0.852	0.494	0.935

Equilibrium sites for atomic lithium in amorphous silicon

Scaled atom positions (a, b, c) and energy ε with respect to the energy of the lowest-energy equilibrium site.

a	b	c	ε
0.677	0.253	0.824	0.36
0.317	0.251	0.565	0.24
0.194	0.539	0.209	0.83
0.963	0.429	0.887	0.60
0.309	0.008	0.885	0.33
0.433	0.572	0.426	0.22
0.469	0.685	0.621	0.13
0.648	0.006	0.565	0.16
0.538	0.952	0.583	0.17
0.490	0.894	0.614	0.16
0.390	0.157	0.167	0.00
0.009	0.196	0.173	0.11
0.175	0.227	0.228	0.01
0.813	0.854	0.770	0.40
0.810	0.902	0.886	0.25
0.479	0.804	0.234	1.35
0.526	0.730	0.038	0.86
0.578	0.871	0.962	1.08
0.134	0.889	0.510	0.31
0.053	0.755	0.674	1.42
0.174	0.667	0.827	0.63
0.171	0.773	0.988	0.28
0.681	0.257	0.393	0.78
0.770	0.331	0.231	1.45
0.934	0.775	0.075	0.14
0.618	0.479	0.090	0.25
0.840	0.688	0.291	0.12
0.795	0.571	0.121	0.09
0.006	0.351	0.602	0.28
0.898	0.466	0.517	0.59
0.849	0.590	0.490	0.36
0.213	0.888	0.275	1.38