Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

Characterization of amorphous Li_xSi structures from ReaxFF via accelerated exploration of local minima

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2 Methods

The crystalline LiSi initial structures extracted from the Materials Proeject are the ones with the following *Materials id*:

- mp-1314: Li12Si7[1–5],
- mp-672287: Li13Si4[2,5–7],
- mp-569849: Li15Si4[2,5,8–10],
- mp-29720: Li21Si5[2,5,11,12].

Li_xSi	N_{Li}	N_{Si}	frames	E_{mean} / N_T [eV]	E_{std} / N_T [eV]	$\sqrt{kT}$ / N_T [eV]
$Li_{0.21}$Si	140	667	774	-4.399	0.003	0.0002
$Li_{0.62}$Si	416	670	1665	-4.002	0.005	0.0001
$Li_{1.25}$Si	839	671	1224	-3.521	0.004	0.0001
$Li_{1.71}$Si	1152	672	2132	-3.286	0.002	0.0001
$Li_{2.17}$Si	693	319	1699	-3.126	0.002	0.0002
$Li_{2.71}$Si	865	319	1504	-2.964	0.002	0.0001
$Li_{3.25}$Si	1040	320	1464	-2.856	0.003	0.0001
$Li_{3.75}$Si	1080	288	2660	-2.777	0.002	0.0001
$Li_{4.20}$Si	1344	320	1600	-2.717	0.001	0.0001

Table 1: Information of the data set. Energies are in eV and the frames are the number of structures used to compute the different graphics in main text.

In table 1 is the information about the data set used to obtain the results of this work.

3 Results and discussion

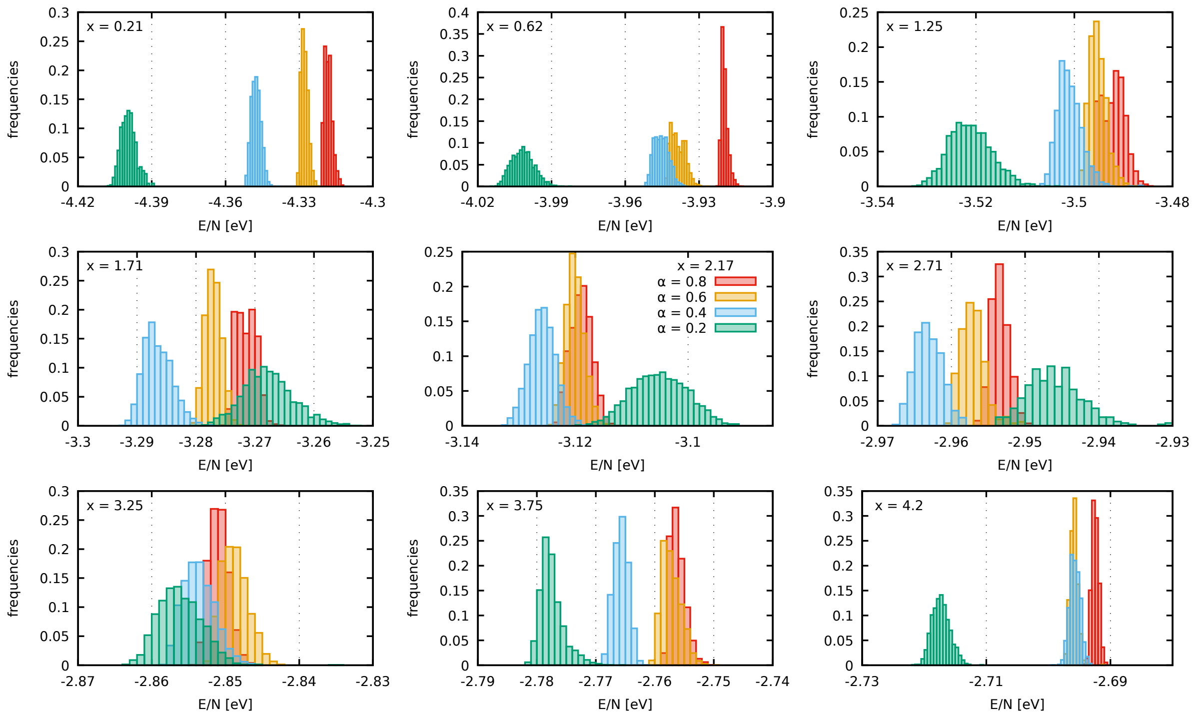


Figure S1: Potential energy histograms after the minimization with conjugated gradient of the structures obtained trough AELM with different values of α for each composition of $Li_x Si$ considered.

x	Formation energy [eV]	Standard deviation [eV]
0.21	0.5027	0.0037
0.62	0.1206	0.0074
1.25	-0.1160	0.0096
1.71	-0.2358	0.0065
2.17	-0.3551	0.0075
2.71	-0.4098	0.0072
3.25	-0.5187	0.0126
3.75	-0.6202	0.0097
4.20	-0.6995	0.0075

Table 2: Formation energy values obtained from equation 3 of the main text.

The formation energy values with their standard deviation as a function of x in $Li_x Si$ are presented in table 2.

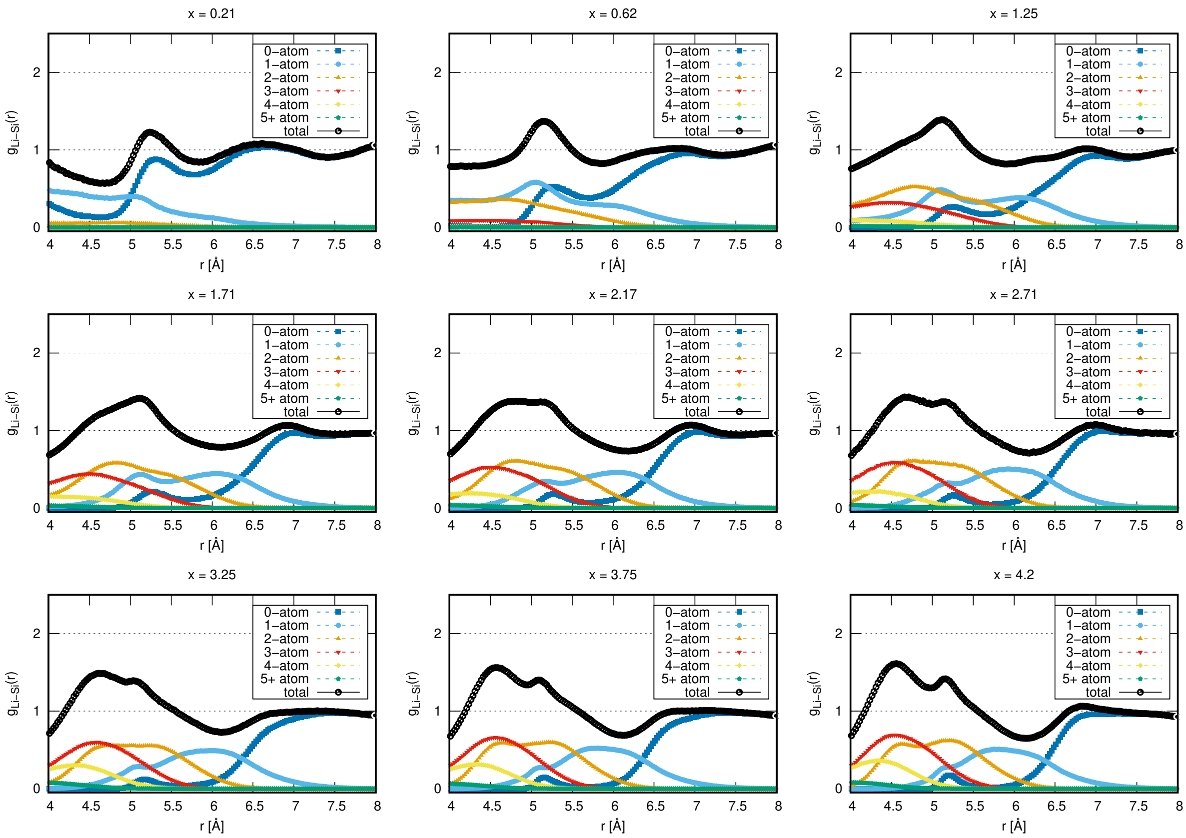
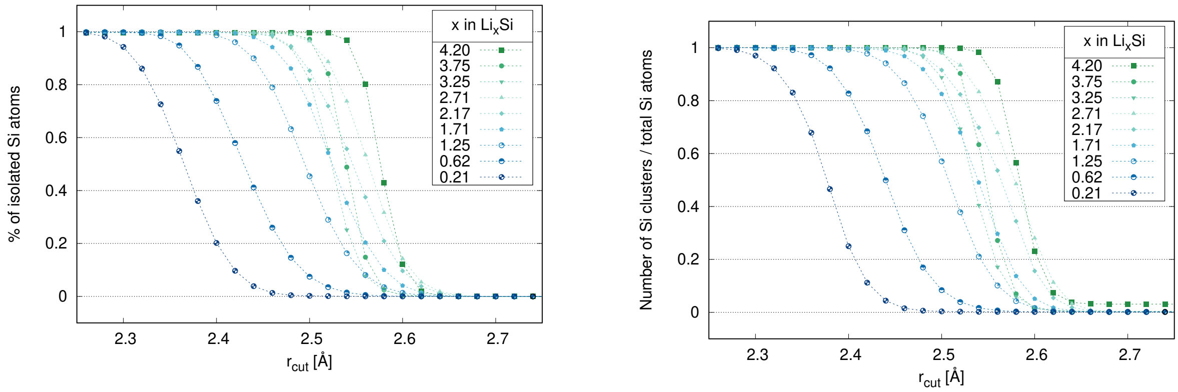


Figure S2: Interconnections of second nearest Li neighbors with a central Si atom for each concentration x of Li_xSi considered. The number of first nearest neighbors connecting second nearest neighbors with the central Si atom is reported in the inset of the figures. In addition to the total RDF_{Li-Si}, each of the contributions corresponding to the different types of possible interconnections is plotted.



(a) Percentage of isolated Si atoms. This is defined as the percentage of Si atoms that lay at at distance from other Si atom larger that r_{cut}. When the cutoff radius is higher that the distance at which the first peak of the RDF_{Si-Si} finishes, there are no isolated Si atoms, rather an a-Si network where all atoms are interconnected.

(b) Ratio between the number of Si clusters and the total number of Si atoms. When the cutoff radius is lower than the first RDF_{Si-Si} peak, the number of clusters is equal to the number of Si atoms, and when the cutoff radius is larger than the first RDF_{Si-Si} peak, there is only one cluster.

Figure S3: Cluster formation indicating an a-Si network.

References

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