Supporting Information
Finite Temperature Behavior of Carbon Atom Doped Silicon Clusters: Depressed Thermal Stabilities, Co-existing isomers, Reversible Dynamical Pathways and Fragmentation Channels.

Krati Joshi[a‡], Ashakiran Maibam[b‡], Sailaja Krishnamurty*[b‡]
[a] *Functional Materials Division, CSIR-Central Electrochemical Research Institute, Karaikudi-630 006, India*
[b] *Physical and Materials Division, CSIR-National Chemical Laboratory, Pune 411 008, India*
[‡] *Academy of Scientific and Innovative Research, CSIR-Human Resource Development Centre (CSIR-HRDC) Campus, Postal Staff College area, Gaziabad, 201 002, Uttar Pradesh, India*

Author Information:

Corresponding author: Sailaja Krishnamurty, e-mail:- sailaja.raaj@gmail.com

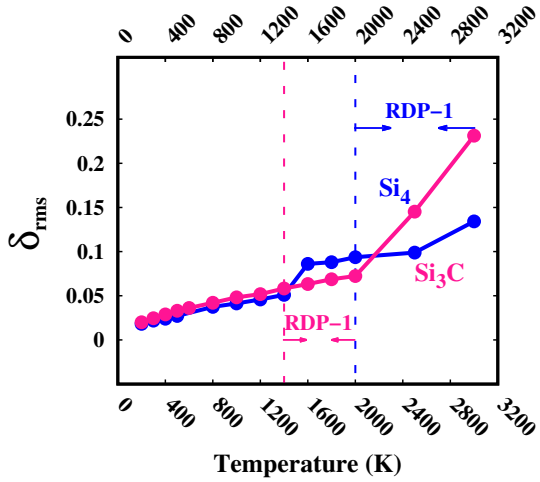

Figure S1. δ_{rms} values for Si_3C and Si_4 clusters at various finite temperatures.

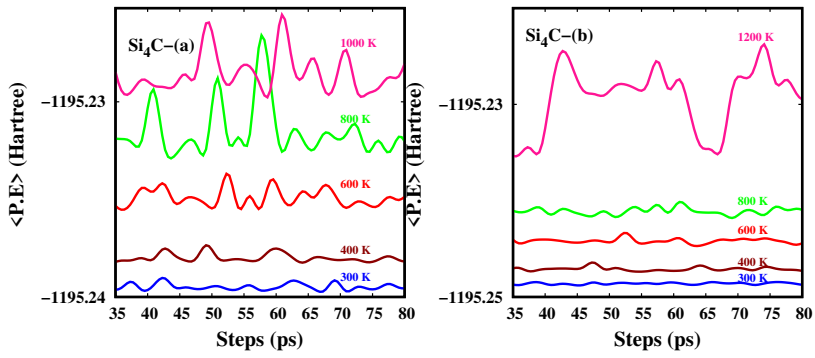

Figure S2. Short-time (1000 steps) averaged potential energies for Si_4C-a and Si_4C-b clusters

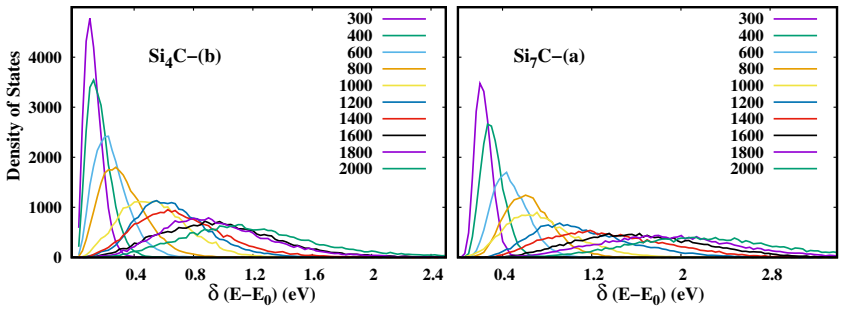

Figure S3. Multi-histograms representing the "density of states" or " probability distribution of potential energies Si_4C-b and Si_7C-a clusters

Figure S3 presents the multi-histograms representing the "density of states" or " probability distribution of potential energies" as a function of temperature for Si_4C–b and Si_7C–a clusters. In case of Si_4C–b, the histogram curve of 300 temperature accesses configurations having energies between 0.05 to 0.38 eV. This energy range has appreciable overlap with curves of 400-800 K temperatures, slight overlap with 1000-1400 K and negligible overlap with the 1600-2000 K curves. On the other hand, in case of Si_7C–a, the curves of 400 K and 600 K have significant overlap with 300 K curve which is accessing the energy states between 0.05 eV-0.4 eV. The histograms of 800 K-1400 K have slight overlap with this energy range, followed by no overlapping with the curves of 1600-2000K. This distribution reaffirms the fact that the starting structure is lost after 800 K and 600 K temperature for Si_4C–b and Si_7C–a clusters, respectively. Additionally, it is noted that the number of energy states acquired by Si_4C–b particularly within 0.05-0.8 eV of energy is much higher as compared to that of Si_7C–a. Also, as the potential energy increases, the histogram curves become more flat and broader for Si_7C–a.

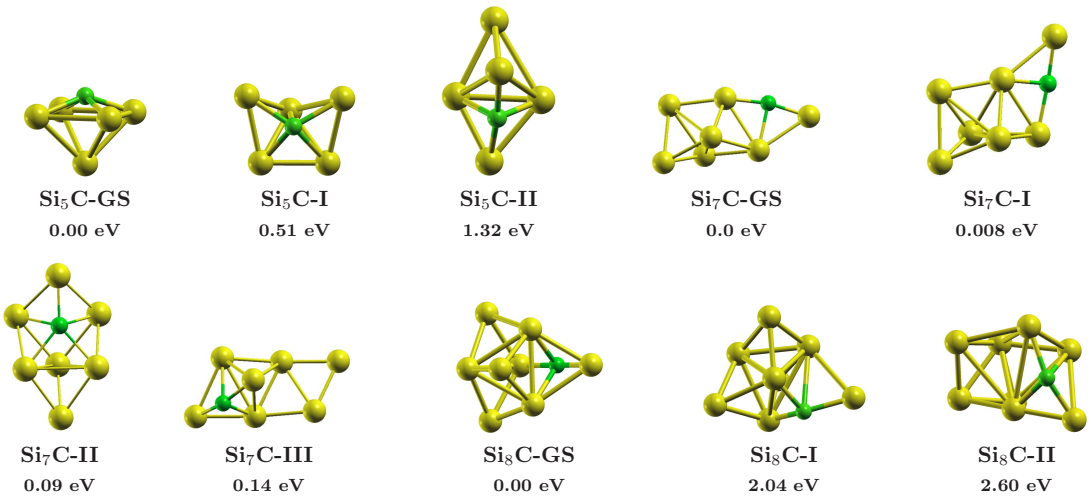

Figure S4. Higher energy conformations of Si_nC clusters with their relative energies (eV) observed at finite temperature

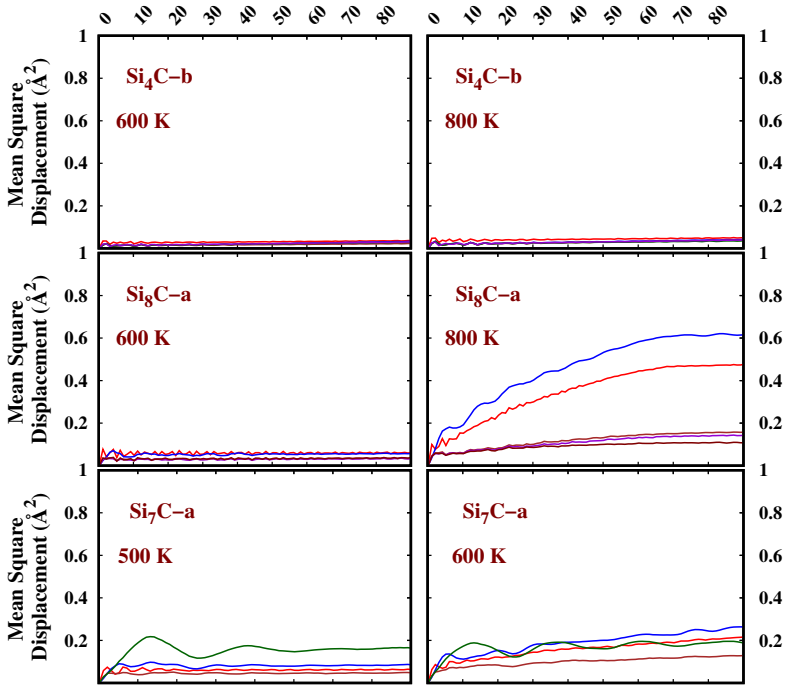

Figure S5. Mean square displacements of atoms in Si_nC clusters at 500, 600 and 800 K temperature.

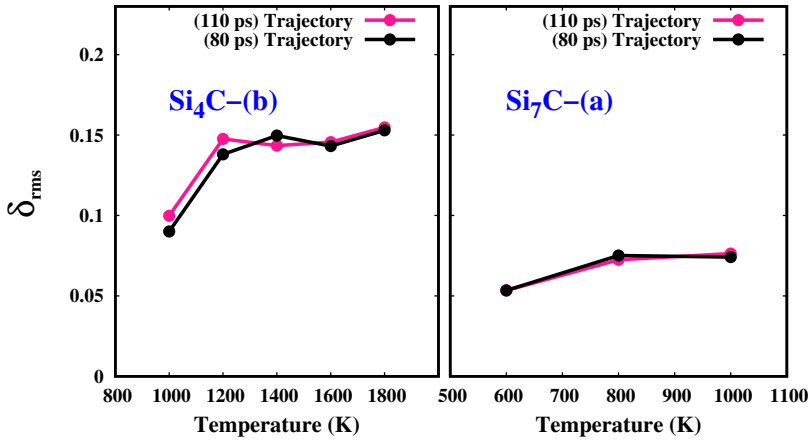

Figure S6. δ_{rms} values for the extended trajectories of Si_4C-b and Si_7C-a clusters at 1000 K, 1200 K, 1400 K, 1600 K, 1800 K (RDP-1) and 600 K, 800 K, 1000 K (RDP-1) temperatures, respectively.

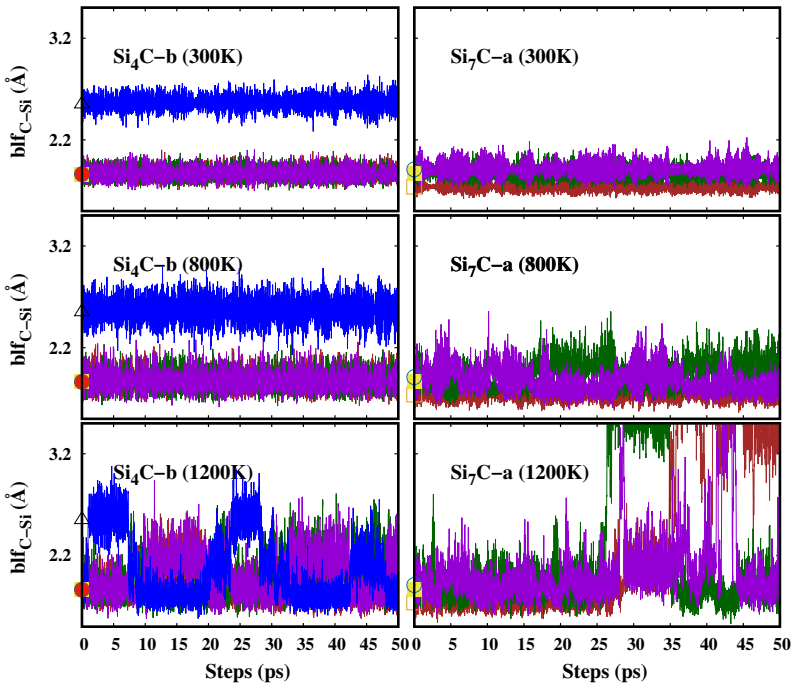

Figure S7. Fluctuations of C-Si interatomic distances as a function of time for Si_4C-b and Si_7C-a clusters. The bullet points in the plots represent corresponding C-Si interatomic bond distances of the starting geometry.

Cartesian coordinates of Si_nC (n=3-8) conformations:

Si_3C-a

C	0.000000	0.000000	0.000000
SI	0.000000	0.000000	1.782403
SI	0.487079	0.000000	-1.715046
SI	1.933958	0.000021	0.267538

Si_4C-a

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.796030
Si	0.000000	0.093741	-1.793588
Si	-0.972833	-1.795644	-0.697398
Si	0.971922	-1.830154	0.602769

Si_4C-b

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.863407
Si	1.827650	0.000000	-0.363540
Si	-0.442620	1.773343	-0.363363
Si	1.401378	1.794135	1.149999

Si_4C-I (b from Figure 4)

C	-0.599785	0.499026	-0.330450
Si	1.538753	0.141257	-0.212287
Si	-0.080017	-1.148559	0.975922
Si	-1.118747	1.081490	1.213197
Si	-0.083485	-0.287601	-1.835512

Si_4C-II (c from Figure 4)

C	0.085290	1.113766	-0.538323
Si	1.563371	0.271265	0.019715
Si	-0.215510	-1.278763	0.682509
Si	-0.955400	0.987957	0.947699
Si	-0.428937	-0.456770	-1.419704

Si_4C-III (d from Figure 4)

C	0.277004	0.216684	0.595519
Si	0.094347	-0.076849	-1.061965
Si	-0.427743	0.107599	2.375583
Si	1.560341	1.102902	-2.075557
Si	-1.345408	-1.226319	0.507260

Si_5C-a

C	0.000000	0.000000	0.00000
SI	0.000000	0.000000	1.86460
SI	0.927718	0.000000	-1.61743
SI	0.635395	-1.813150	0.16928
SI	0.635395	1.813150	0.16928
SI	2.191357	0.000000	0.58384

Si_5C-b

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.914461
Si	1.171274	0.000000	-1.514361
Si	0.585772	1.811643	0.200096
Si	0.585604	-1.811720	0.200033
Si	2.162000	-0.000111	0.738524

Si_5C-I (Figure S4)

C	-0.106397	0.149051	0.824737
SI	1.132632	-1.273714	0.162754
SI	-1.595721	1.111746	0.096440
SI	1.603084	1.013884	0.657904
SI	0.057699	0.276862	-1.392802
SI	-1.152194	-1.192528	0.122990

Si_5C-II (Figure S4)

C	0.008023	-0.218782	1.071393
SI	1.293503	-0.626402	-0.238005
SI	-1.274161	-0.324962	-0.468111
SI	-0.462919	-1.956330	0.834525
SI	0.306196	1.523084	1.106510
SI	0.133951	1.478178	-1.693125

Si_6C-a

C	0.000000	0.000000	0.000000
SI	0.000000	0.000000	2.055769
SI	1.934351	0.000000	0.696051
SI	1.280990	-0.568862	-1.503966
SI	-1.057189	-0.920260	-1.503971
SI	-1.848859	-0.568863	0.696103

Si_6C-I (b from Figure 8)

C	0.066888	1.113209	0.323814
SI	1.165239	1.667501	-1.107486
SI	1.568950	-0.326584	-0.018544
SI	0.388739	-2.328962	0.203860
SI	-0.684992	-0.243436	-1.186120
SI	-1.777458	1.330645	0.658572

SI	0.309644	-2.060365	0.440504	SI	-0.679940	-0.584953	1.330394
Si_6C-II (c from Figure 8)				**Si_6C-III (d from Figure 8)**			
C	-0.996889	0.081231	0.054174	C	-0.082193	0.637385	-0.652488
SI	0.617148	0.081280	-1.267678	SI	0.176542	-1.758492	0.872734
SI	1.698599	-1.776425	-0.161190	SI	-1.247435	-0.883254	-1.185142
SI	-0.759700	-1.801022	-0.055423	SI	-0.148419	2.359503	0.051494
SI	-2.134318	1.517646	0.176282	SI	1.185818	-0.726554	-1.350152
SI	0.279208	2.007940	0.100723	SI	1.298984	0.457678	0.874044
SI	0.724872	-0.050533	1.224776	SI	-1.211571	0.294350	1.043885
Si_7C-a				**Si_7C-b**			
C	0.000000	0.000000	0.000000	C	0.000000	0.000000	0.000000
SI	0.000000	0.000000	1.739839	SI	0.000000	0.000000	1.738353
SI	0.000000	0.311449	-1.842250	SI	0.409665	0.000000	-1.743222
SI	1.180958	1.498951	0.078564	SI	1.951056	0.464197	0.157717
SI	3.066102	2.669294	-0.591567	SI	1.137074	0.666121	-3.816800
SI	0.478646	2.814950	-1.811979	SI	2.719989	-0.716760	-1.933200
SI	2.471979	3.117379	-3.030983	SI	3.584626	0.915018	-3.396773
SI	2.322654	0.927042	-2.181402	SI	2.140056	1.883862	-1.802807
Si_7C-I (Figure S4)				**Si_7C-II (Figure S4)**			
C	0.000000	0.000000	0.000000	C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.739839	Si	0.000000	0.000000	2.053402
Si	0.000000	0.311449	-1.842250	Si	1.977495	0.000000	0.635373
Si	1.180958	1.498951	0.078564	Si	0.250688	1.593114	-1.312438
Si	3.066102	2.669294	-0.591567	Si	0.865761	-0.802495	-1.427258
Si	0.478646	2.814950	-1.811979	Si	-1.475691	1.401013	0.366326
Si	2.471979	3.117379	-3.030983	Si	-0.833496	2.275228	2.580954
Si	2.322654	0.927042	-2.181402	Si	0.867436	2.220501	1.048775
Si_7C-III (Figure S4)				**Si_8C-a**			
C	0.000000	0.000000	0.000000	C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.788803	SI	0.000000	0.000000	1.787863
Si	0.629104	0.000000	-1.766032	SI	0.000000	0.094597	-1.854562
Si	0.940861	-1.699445	-0.166599	SI	-1.965298	1.451796	-2.097926
Si	1.964663	0.705091	0.307208	SI	-1.382527	1.536359	0.243497
Si	2.725233	-1.339525	1.441943	SI	1.962725	1.455673	-2.097832
Si	3.108634	-2.993528	2.925757	SI	1.379665	1.539207	0.243319
Si	1.107196	-3.180165	1.724631	SI	-0.003356	3.491955	0.594089
				SI	-0.002794	2.857339	-1.736894
Si_8C-b				**Si_8C-I (Figure S4)**			
C	0.000000	0.000000	0.000000	C	1.121067	0.643310	-1.120416
SI	0.000000	0.000000	1.814750	Si	2.357378	-0.666777	-1.691305
SI	0.891500	0.000000	-1.688200	Si	-0.654629	0.084525	-1.417285

SI	-0.597869	-1.661203	-0.803419	Si	-1.582336	-1.790169	-0.448860
SI	1.948581	-0.672522	0.335332	Si	0.654021	-1.504906	0.323667
SI	-1.021410	-3.779771	0.228627	Si	-1.681123	1.973080	-0.167919
SI	0.273816	-2.627877	1.841951	Si	0.690210	1.551316	0.408014
SI	2.620452	-2.821207	1.387996	Si	0.980343	0.124287	2.196511
SI	1.239211	-3.377540	-0.406062	Si	-1.243297	-0.046473	1.276333

Si_8C-II (Figure S4)

C	-0.696634	1.282243	1.435483
Si	0.944606	2.154565	1.607493
Si	-1.460541	-1.986586	0.172822
Si	-2.195967	0.659732	0.377833
Si	2.038434	-0.367360	-1.459836
Si	-0.328514	1.809229	-1.010760
Si	0.757750	-0.033149	1.117644
Si	0.911309	-2.081488	0.108472
Si	-0.369156	-0.703305	-1.527565