

## Supporting Information

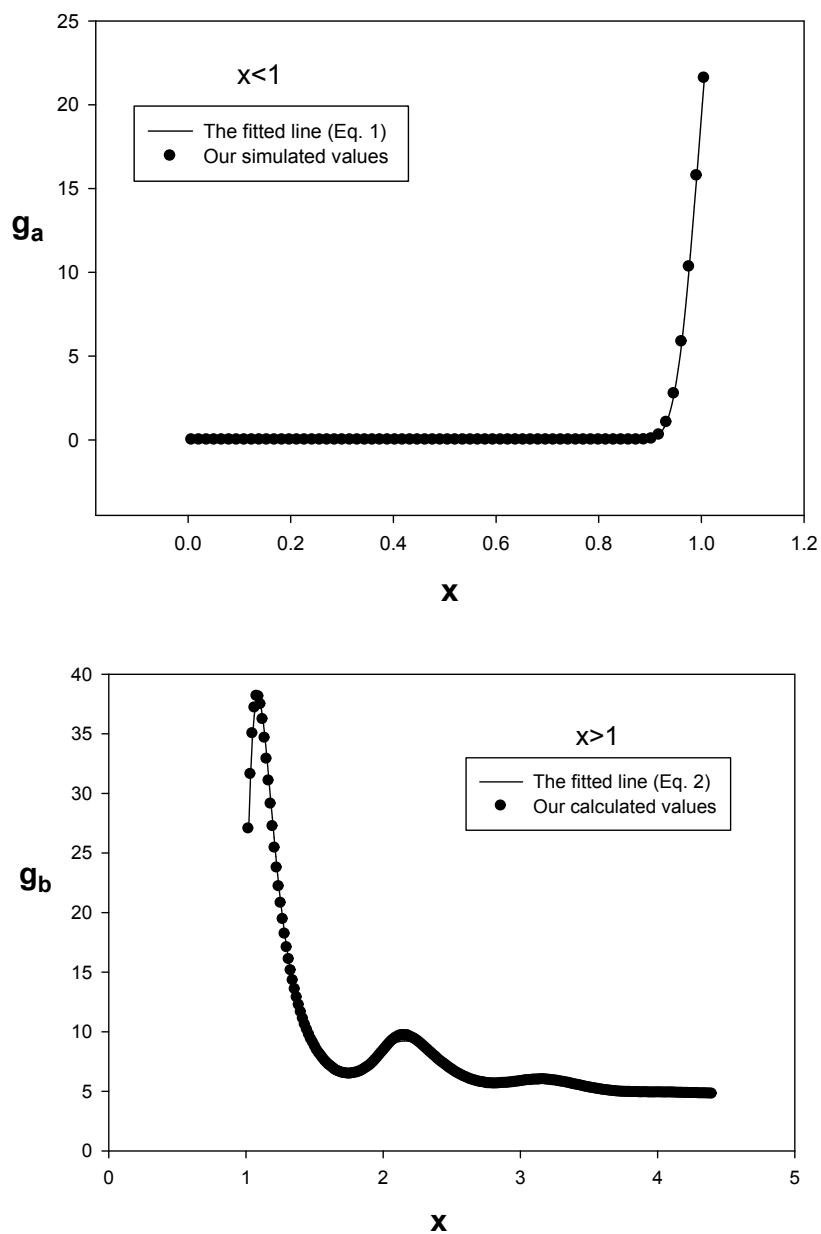
### 1- Details of the fitting

We have calculated the Ar-Ar and Ar-C RDFs of the confined atoms into the (33,0) CNT as a function of reduced separation in the reduced temperature and density ranges from  $5.2 \leq T^* \leq 10.4$  and  $1.58 \leq \rho_{\text{mix}}^* \leq 1.66$  using the MD simulation. Then, we have fitted the calculated RDFs at two ranges of the reduced separation ( $x$ ) to the following equations using the Sigmaplot software:<sup>26</sup>

$$g_a = s \exp\left[-\left(m x + n\right)^4\right] \quad x \leq 1 \quad (1)$$

$$g_b = 1 + (x)^{-4} \exp\left[-\left(a x + b\right)\right] \sin\left[\left(c x + d\right)\right] + (x)^{-4} \exp\left[-\left(q x + h\right)\right] \cos\left[\left(k x + l\right)\right] \quad x > 1 \quad (2)$$

where  $g$  represents the RDF and  $a, b, c, d, q, h, k, l, m, n,$  and  $s$  are the adjustable parameters. In order to fit the data using the Sigmaplot, it is necessary to define Eqs. (1) and (2) in the "User defined" section in the "Dynamic fit wizards". The  $R^2$  values can be checked in a report page. Figure S1 shows the fitted lines for the Ar-Ar RDF on the two different ranges of  $x$ :



**Fig. S1.** Comparison between the fitted line and the simulated data at two different ranges of  $x$ .

The adjustable parameters  $a$ ,  $b$ ,  $c$ ,  $d$ ,  $q$ ,  $h$ ,  $k$ ,  $l$ ,  $m$ ,  $n$ , and  $s$  and their values along with the  $R^2$  values for the Ar-Ar and Ar-C RDFs have been presented in Tables S1 and S2.

**Table S1.** The values of the parameters of the Eqs. (1) and (2) for the Ar-Ar RDFs.

$T^*$	$\rho_{\text{mix}}^*$	$s_1$	$m_1$	$n_1$	$R^2$	$a_1$	$b_1$	$c_1$	$d_1$	$q_1$	$h_1$	$k_1$	$l_1$	$R^2$
5.2015	1.6181	22.6225	-6.0165	6.6844	1.0000	-0.6598	-4.6476	27.1831	-31.3309	2.4231	-6.4151	-235.0714	-432.7753	0.9988
	1.6001	23.2819	-6.0188	6.6840	1.0000	-0.7183	-4.4130	30.3193	-33.4924	2.0477	-5.8316	-261.0638	-1850.3089	0.9985
	1.5908	24.1053	-6.0314	6.6925	1.0000	-0.7708	-4.2262	32.6537	-34.6715	1.6318	-5.2335	-279.5751	-755.8057	0.9982
	1.5887	25.0328	-6.0887	6.7404	1.0000	-0.8138	-4.0837	34.2347	-35.0565	1.2710	-4.7362	-294.1401	-25.2097	0.9979
	1.5932	26.2003	-6.1229	6.7669	1.0000	-0.8645	-3.9202	35.7223	-34.9148	0.8718	-4.1903	307.0182	376.8611	0.9977
	1.6026	27.5087	-6.1833	6.8162	1.0000	-0.8987	-3.8151	36.6360	-34.6579	0.6141	-3.8650	315.8194	-347.5829	0.9973
	1.6170	28.7922	-6.2724	6.8891	1.0000	-0.9374	-3.6964	37.4995	-34.1217	0.3672	-3.5559	-322.8414	-2170.1259	0.9970
	1.6354	30.4110	-6.3255	6.9290	1.0000	-0.9668	-3.6091	38.1574	-33.7208	0.2228	-3.3997	-329.2725	-3248.2696	0.9966
1.6606	32.0804	6.4395	-7.0227	1.0000	-1.0030	-3.4998	38.8002	-32.9728	0.0829	-3.2473	336.1250	2166.4949	0.9961	
6.0684	1.6181	21.9007	-5.8712	6.5069	1.0000	-0.7447	-4.3119	31.6378	-34.6072	2.0753	-5.7829	-245.6586	-1505.6558	0.9991
	1.6001	22.6195	-5.8857	6.5152	1.0000	-0.7727	-4.2219	32.8859	-35.1092	1.7973	-5.3863	-261.4435	306.7104	0.9989
	1.5908	23.5049	-5.9313	6.5527	1.0000	-0.8176	-4.0728	-34.4969	-144.5823	1.4213	-4.8511	279.4265	-320.6450	0.9987
	1.5887	24.5491	-5.9607	6.5741	1.0000	-0.8659	-3.9152	35.7372	-34.9160	0.9821	-4.2387	295.7207	-332.5120	0.9984
	1.5932	25.7222	-6.0050	6.6090	1.0000	-0.8900	-3.8445	36.7415	-34.8554	0.7730	-3.9847	304.4112	-337.4376	0.9982
	1.6026	26.9941	-6.0730	6.6643	1.0000	-0.9209	-3.7505	37.1930	-34.4446	0.5366	-3.6922	-313.6461	342.5997	0.9980
	1.6170	28.3287	-6.1371	6.7147	1.0000	-0.9522	-3.6555	37.8447	-33.9236	0.3401	-3.4553	-320.0493	-6855.6981	0.9976

	1.6354	29.7361	-6.2434	6.8014	1.0000	-0.9803	-3.5706	38.3912	-33.4126	0.2044	-3.3104	327.2975	-347.0998	0.9972
	1.6606	31.2151	-6.3518	6.8892	1.0000	0.0894	-3.1961	-334.2331	439.6292	-1.0090	-3.4844	38.8979	-122.8196	0.9967
6.9353	1.6181	21.4429	-5.7457	6.3510	1.0000	-0.7859	-4.1722	33.4069	-35.4499	1.8371	-5.3651	-248.1305	-4746.5680	0.9993
	1.6001	22.2669	-5.7585	6.3597	1.0000	-0.8011	-4.1319	34.1397	-35.7616	1.6682	-5.1461	-260.8842	303.8199	0.9992
	1.5908	23.1828	-5.8252	6.4149	1.0000	-0.8481	-3.9774	35.4369	-35.3715	1.2173	-4.5012	-279.6546	-402.3562	0.9989
	1.5887	24.1985	-5.8709	6.4501	1.0000	-0.8775	-3.8861	36.2383	-35.1274	0.9577	-4.1574	-292.4668	-5433.2295	0.9987
	1.5932	25.2820	-5.9351	6.5020	1.0000	-0.9086	-3.7910	36.9559	-34.6768	0.6943	-3.8168	-302.9788	-1826.5382	0.9985
	1.6026	26.5589	-6.0047	6.5586	1.0000	-0.9391	-3.6974	37.5815	-34.1294	0.4648	-3.5324	310.8132	1823.2281	0.9983
	1.6170	27.8457	6.0727	-6.6111	1.0000	-0.9607	-3.6329	38.0426	-33.7900	0.3379	-3.3985	-318.4218	-3979.4084	0.9980
	1.6354	29.1668	-6.1754	6.6947	1.0000	-0.9861	-3.5560	38.4992	-33.2682	0.2062	-3.2607	325.5334	-343.4209	0.9975
	1.6606	30.5279	-6.2979	6.7936	1.0000	-1.0111	-3.4805	38.9487	-32.7808	0.1009	-3.1605	-332.9361	346.8543	0.9971
7.8022	1.6181	21.1908	-5.6491	6.2285	0.9999	-0.8159	-4.0787	34.4758	-35.5816	1.6163	-4.9805	-251.5990	-1146.6514	0.9994
	1.6001	21.9680	-5.7022	6.2716	0.9999	1.4341	-4.7434	262.4793	-571.2965	-0.8345	-4.0239	-35.2041	125.7621	0.9993
	1.5908	22.9353	-5.7456	6.3053	1.0000	1.1693	-4.3767	278.6393	-584.4128	-0.8638	-3.9320	35.9738	-125.4269	0.9992
	1.5887	24.0226	-5.7684	6.3222	1.0000	-0.8917	-3.8469	36.6608	-35.0578	0.8933	-4.0190	-290.8986	-1837.0832	0.9990
	1.5932	25.0193	-5.8634	6.3998	1.0000	-0.9148	-3.7765	37.1699	-34.6772	0.6926	-3.7727	-300.6530	-1470.7598	0.9988
	1.6026	26.1638	-5.9398	6.4608	1.0000	-0.9435	-3.6872	37.7122	-34.0989	0.4791	-3.5070	-309.0219	-2546.6998	0.9986
	1.6170	27.3429	-6.0338	6.5361	1.0000	-0.9644	-3.6244	38.1281	-33.7186	0.3453	-3.3638	-316.3318	-5423.2706	0.9983
	1.6354	28.6778	-6.1213	6.6060	1.0000	-0.9881	-3.5517	38.5386	-33.2135	0.2210	-3.2364	-324.6003	-2898.9101	0.9978

	1.6606	29.9590	-6.2369	6.6990	1.0000	-1.0114	-3.4813	38.9533	-32.7510	0.1218	-3.1443	-331.3000	-6496.3207	0.9973
8.6691	1.6181	21.0174	-5.5216	6.0813	0.9999	-0.8260	-4.0539	35.0491	-35.9780	1.5541	-4.8677	248.2820	1151.9882	0.9996
	1.6001	21.7819	-5.6222	6.1671	0.9999	-0.8490	-3.9820	-35.6523	215.6749	1.3013	-4.5197	263.5169	-660.0743	0.9994
	1.5908	22.7299	-5.6803	6.2139	0.9999	-0.8757	-3.8984	36.3186	-35.3293	1.0866	-4.2203	-277.2146	-769.4935	0.9992
	1.5887	23.7179	-5.7381	6.2596	1.0000	-0.9018	-3.8188	36.9291	-34.9342	0.8348	-3.8960	-289.0792	-5080.9997	0.9991
	1.5932	24.7688	-5.7990	6.3078	1.0000	-0.9242	-3.7492	37.3618	-34.4652	0.6461	-3.6628	-298.4657	324.6539	0.9989
	1.6026	25.8677	-5.8688	6.3622	1.0000	-0.9483	-3.6758	37.8439	-34.0382	0.4791	-3.4662	-307.4811	-749.8593	0.9986
	1.6170	26.9565	-5.9792	6.4520	1.0000	-0.9685	-3.6142	38.2280	-33.6565	0.3464	-3.3267	-315.4035	-9025.4595	0.9984
	1.6354	28.2630	-6.0653	6.5204	1.0000	-0.9896	-3.5494	38.5958	-33.2175	0.2395	-3.2200	-322.6206	-8662.3282	0.9980
	1.6606	29.4537	-6.1905	6.6216	1.0000	-1.0117	-3.4821	38.9652	-32.7484	0.1391	-3.1276	-330.4651	-6498.2005	0.9974
9.5360	1.6181	20.7208	-5.5383	6.0666	0.9999	1.5401	-4.8055	246.6743	-554.8033	-0.8336	-4.0337	-35.3533	126.0668	0.9997
	1.6001	21.6179	-5.5814	6.1010	0.9999	-0.8571	-3.9616	36.0029	-35.8136	1.3004	-4.4777	261.0251	1504.0059	0.9995
	1.5908	22.5387	-5.6328	6.1413	0.9999	-0.8825	-3.8826	36.5828	-35.3564	1.0281	-4.1106	-274.8592	-413.9185	0.9994
	1.5887	23.4938	-5.6940	6.1896	0.9999	-0.9084	-3.8003	37.0643	-34.7729	0.8133	-3.8239	-287.4908	-1124.6479	0.9992
	1.5932	24.5124	-5.7500	6.2328	0.9999	-0.9301	-3.7342	37.5296	-34.4237	0.6380	-3.6122	-296.8322	-5078.5215	0.9990
	1.6026	25.6345	-5.8212	6.2896	1.0000	-0.9506	-3.6712	37.9126	-34.0133	0.4849	-3.4418	306.4633	32.1215	0.9988
	1.6170	26.7043	-5.9254	6.3734	1.0000	-0.9682	-3.6175	38.2511	-33.6885	0.3758	-3.3327	-314.1994	-2907.9083	0.9985
	1.6354	27.8085	-6.0437	6.4689	1.0000	-0.9890	-3.5531	38.6013	-33.2441	0.2588	-3.2131	-321.6034	-1464.2913	0.9981
	1.6606	29.0168	-6.1558	6.5579	1.0000	-1.0110	-3.4857	38.9585	-32.7598	0.1555	-3.1126	-329.2275	-2180.5474	0.9976

10.4029	1.6181	20.6114	-5.4907	5.9982	0.9999	-0.8482	-3.9910	35.8080	-35.9486	1.4061	-4.5775	248.5586	1155.9999	0.9997
	1.6001	21.4759	-5.5388	6.0364	0.9999	-0.8695	-3.9252	36.3309	-35.6395	1.1969	-4.2936	-261.2070	-1146.3978	0.9995
	1.5908	22.3675	-5.5872	6.0741	0.9999	-0.8909	-3.8581	36.7839	-35.1929	0.9658	-3.9879	272.9608	-301.9043	0.9994
	1.5887	23.3211	-5.6334	6.1097	0.9999	-0.9086	-3.8040	37.1670	-34.8969	0.8202	-3.8140	-284.1443	-1849.4827	0.9992
	1.5932	24.3370	-5.6950	6.1566	0.9999	-0.9288	-3.7422	37.5839	-34.5439	0.6632	-3.6258	-294.6766	-6521.8356	0.9991
	1.6026	25.2927	-5.8007	6.2425	1.0000	-0.9486	-3.6802	37.9255	-34.1112	0.5120	-3.4525	-304.1801	-2915.3945	0.9989
	1.6170	26.3979	-5.8868	6.3103	1.0000	-0.9682	-3.6191	38.2598	-33.6840	0.3934	-3.3236	-312.0645	-1471.3047	0.9985
	1.6354	27.4572	-6.0048	6.4050	1.0000	0.2756	-3.2052	-321.0175	424.3468	-0.9889	-3.5550	38.6222	-123.2750	0.9982
	1.6606	28.6006	-6.1269	6.5028	1.0000	-1.0099	-3.4901	38.9668	-32.8316	0.1742	-3.1056	-329.2318	-380.9657	0.9976

**Table S2.** The values of the parameters of the Eqs. (1) and (2) for the Ar-C(CNT) RDFs.

$T^*$	$\rho_{\text{mix}}^*$	$s_1$	$m_1$	$n_1$	$R^2$	$a_1$	$b_1$	$c_1$	$d_1$	$q_1$	$h_1$	$k_1$	$l_1$	$R^2$
5.2015	1.6181	4.6634	-5.0863	5.8911	1.0000	-0.8983	-3.2222	32.2161	-33.1807	0.2902	-1.7641	-236.3780	-78.0274	0.9993
	1.6001	4.5211	-5.0695	5.8718	1.0000	-0.9442	-3.0693	33.4474	-34.5648	0.2016	-1.6601	-239.8518	-1874.8552	0.9982
	1.5908	4.3900	-5.1077	5.9028	1.0000	-0.9828	-2.9435	34.3969	-35.7283	0.1739	-1.6524	-244.3495	-70.1762	0.9959
	1.5887	4.3092	-5.1397	5.9276	1.0000	-1.0159	-2.8357	35.1743	-36.5818	0.1424	-1.6147	250.6852	1863.4650	0.9910
	1.5932	4.2287	-5.1851	5.9624	1.0000	-1.0448	-2.7425	35.8412	-37.3289	0.0995	-1.5679	-257.5116	303.5524	0.9820
	1.6026	4.2607	-5.1701	5.9436	1.0000	-1.0697	-2.6614	36.3874	-37.8031	0.0690	-1.5192	265.7982	47.7778	0.9701
	1.6170	4.2920	-5.2135	5.9767	1.0000	-1.0926	-2.5869	36.9003	-38.1805	0.0243	-1.4541	-275.5201	-3637.6099	0.9557
	1.6354	4.3217	-5.2709	6.0201	1.0000	-1.1232	-2.4864	37.4736	-38.2407	-0.0862	-1.2634	290.6106	-698.9491	0.9404
1.6606	4.4020	-5.3154	6.0504	1.0000	-1.1459	-2.4128	37.9404	-38.3192	-0.1688	-1.1291	-302.0476	350.4546	0.9277	
6.0684	1.6181	4.2638	-4.8767	5.6697	0.9999	0.1899	-1.5476	230.2825	-542.3151	-0.9472	-3.0619	33.4050	235.4479	0.9988
	1.6001	4.1594	-4.8923	5.6790	0.9999	-0.9817	-2.9489	34.3022	-35.6386	0.1336	-1.5027	-233.4589	-8364.7824	0.9973
	1.5908	4.1094	-4.9069	5.6886	0.9999	-1.0134	-2.8458	35.0540	-36.4921	0.1095	-1.4848	-240.0111	-1157.6797	0.9941
	1.5887	4.0561	-4.9498	5.7218	1.0000	-1.0330	-2.7832	35.5575	-37.2176	0.1172	-1.5365	243.9107	793.7926	0.9894
	1.5932	4.0589	-4.9827	5.7468	0.9999	-1.0576	-2.7031	36.1299	-37.8104	0.1116	-1.5398	-251.6692	-1144.9124	0.9804
	1.6026	4.0825	-5.0102	5.7654	1.0000	-1.0766	-2.6416	36.5443	-38.2103	0.0942	-1.5202	-259.4212	-1137.0979	0.9698
	1.6170	4.1170	-5.0638	5.8066	1.0000	-1.0971	-2.5744	36.9830	-38.4737	0.0654	-1.4755	269.9432	1845.6319	0.9570

	1.6354	4.1698	-5.1079	5.8369	0.9999	-1.1158	-2.5131	37.3735	-38.6097	0.0135	-1.3954	-280.6385	-1114.4882	0.9447
	1.6606	4.2597	-5.1651	5.8791	1.0000	-1.1359	-2.4471	37.7789	-38.6447	-0.0616	-1.2788	293.5361	-339.0225	0.9319
6.9353	1.6181	4.0068	-4.7114	5.4938	0.9999	-0.9794	-2.9572	34.1455	-35.3316	0.0977	-1.3321	-227.1680	-1174.4642	0.9981
	1.6001	3.9453	-4.7157	5.9430	0.9999	-1.0066	-2.8694	34.8389	-36.2412	0.0633	-1.3307	230.9017	-628.8595	0.9963
	1.5908	3.9195	-4.7528	5.5227	0.9999	-1.0278	-2.8015	35.3780	-37.0446	0.0951	-1.4305	-234.1906	272.8136	0.9933
	1.5887	3.9289	-4.7797	5.5425	0.9999	-1.0482	-2.7354	35.8501	-37.6011	0.1085	-1.4772	-240.5800	-2959.3337	0.9884
	1.5932	3.9091	-4.8294	5.5798	0.9999	-1.0649	-2.6818	36.2739	-38.1546	0.1069	-1.5039	-246.3151	-73.4049	0.9806
	1.6026	3.9482	-4.8645	5.6049	0.9999	-1.0797	-2.6337	36.6095	-38.4947	0.1124	-1.5260	253.7978	2225.5069	0.9721
	1.6170	4.0257	-4.8809	5.6126	0.9999	-1.0957	-2.5811	36.9919	-38.7866	0.1135	-1.5332	-263.4526	-1855.0939	0.9607
	1.6354	4.0992	-4.9323	5.6501	0.9999	-1.1112	-2.5299	37.3211	-38.9054	0.0814	-1.4838	-273.3701	-7604.7360	0.9493
	1.6606	4.1847	-4.9856	5.6876	0.9999	-1.1319	-2.4615	37.7252	-38.8739	0.0120	-1.3645	287.7784	1109.1596	0.9366
7.8022	1.6181	3.8038	-4.5814	5.3538	0.9999	-1.0034	-2.8807	34.6747	-35.9942	0.0163	-1.1711	-220.9461	614.3017	0.9996
	1.6001	3.7912	-4.5952	5.3625	0.9999	-1.0227	-2.8189	35.1732	-36.7311	0.0571	-1.2882	226.7019	1178.3451	0.9958
	1.5908	3.7962	-4.6148	5.3758	0.9999	-1.0394	-2.7657	35.6016	-37.3823	0.0716	-1.3639	-229.4696	-95.1481	0.9932
	1.5887	3.7682	-4.6778	5.4260	0.9999	-1.0569	-2.7093	36.0544	-37.9987	0.0935	-1.4336	-235.0944	-808.4147	0.9879
	1.5932	3.8401	-4.6692	5.4131	0.9999	-1.0679	-2.6743	36.3405	-38.4339	0.1125	-1.4976	240.5556	5482.7807	0.9823
	1.6026	3.8713	-4.7393	5.4689	0.9999	-1.0803	-2.6336	36.6472	-38.7239	0.1360	-1.5458	-248.4048	-1513.7122	0.9741
	1.6170	3.9224	-4.7888	5.5045	0.9999	-1.0945	-2.5869	36.9647	-38.9553	0.1325	-1.5502	257.4558	-296.3440	0.9646
	1.6354	4.0196	-4.8224	5.5261	0.9999	-1.1059	-2.5489	37.2276	-39.0769	0.1300	-1.5487	-266.8561	-1133.8177	0.9548

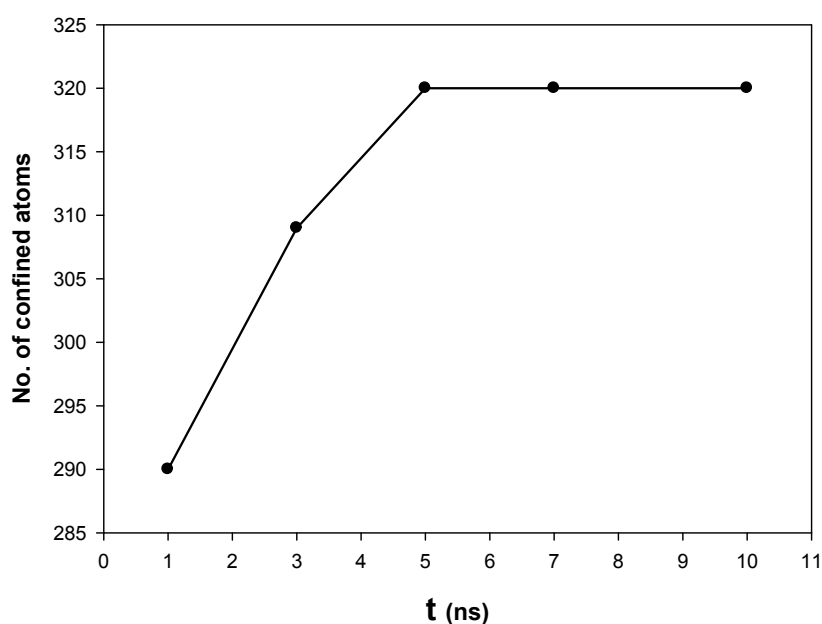


	1.6606	4.1154	-4.8581	5.5477	0.9999	-1.1240	-2.4885	37.5926	-39.0839	0.0906	-1.4758	-279.8460	-39.7152	0.9418
8.6691	1.6181	3.6369	-4.4668	5.2299	0.9999	-1.0188	-2.8328	34.9970	-36.4693	-0.0140	-1.1000	-216.0504	-834.9509	0.9973
	1.6001	3.6535	-4.4867	5.2441	0.9999	-1.0329	-2.7876	35.3736	-37.0611	0.0209	-1.2103	-221.0440	-1548.2956	0.9959
	1.5908	3.6526	-4.5366	5.2835	0.9999	-1.0471	-2.7420	35.7577	-37.6434	0.0492	-1.3063	225.3063	462.4640	0.9931
	1.5887	3.6780	-4.5441	5.2842	0.9999	-1.0605	-2.6996	36.1225	-38.2361	0.0823	-1.4028	-229.4016	-8017.6841	0.9892
	1.5932	3.7355	-4.5847	5.3154	0.9999	-1.0680	-2.6757	36.3610	-38.6589	0.1350	-1.5278	-235.5607	-450.2470	0.9842
	1.6026	3.7928	-4.6173	5.3373	0.9999	-1.0803	-2.6352	36.6450	-38.9187	0.1411	-1.5499	-243.1803	-1161.9675	0.9776
	1.6170	3.8802	-4.6357	5.3458	0.9999	-1.0929	-2.5936	36.9482	-39.1361	0.1613	-1.5808	-252.1142	-5111.6592	0.9686
	1.6354	3.9719	-4.6899	5.3858	0.9999	-1.1061	-2.5492	37.2434	-39.2280	0.1645	-1.5841	-263.3955	-1858.9276	0.9584
	1.6606	4.0566	-4.7621	5.4398	0.9999	-1.1193	-2.5050	37.5140	-39.2363	0.1422	-1.5457	275.1089	46.4807	0.9471
9.5360	1.6181	3.5457	-4.3610	5.1177	0.9999	-1.0239	-2.8181	35.0829	-36.7060	-0.0409	-1.0551	-209.4966	-1926.7072	0.9975
	1.6001	3.5564	-4.3974	5.1468	0.9999	-1.0409	-2.7638	35.5618	-37.4448	1.9000e-3	-1.1867	-216.1281	-4796.9733	0.9954
	1.5908	3.5841	-4.4043	5.1469	0.9999	-1.0544	-2.7206	35.9070	-37.9587	0.0282	-1.2681	-220.2756	-1191.3487	0.9936
	1.5887	3.6202	-4.4508	5.1831	0.9999	-1.0605	-2.7014	36.1264	-38.3983	0.0838	-1.4054	-224.7346	254.4144	0.9900
	1.5932	3.6506	-4.5021	5.2216	0.9999	-1.0713	-2.6662	36.4077	-38.7846	0.1166	-1.4852	-231.5935	-7296.9111	0.9860
	1.6026	3.7347	-4.5224	5.2332	0.9999	-1.0805	-2.6360	36.6531	-39.0631	0.1676	-1.5757	239.3209	1527.7387	0.9798
	1.6170	3.8212	4.5494	-5.2494	0.9999	-1.0917	-2.5986	36.9267	-39.2666	0.1860	-1.6122	-248.0225	-4397.7658	0.9723
	1.6354	3.8857	-4.6313	5.3124	0.9999	-1.1016	-2.5654	37.1521	-39.3459	0.2008	-1.6343	257.6765	-293.1049	0.9632
	1.6606	4.0021	-4.6645	5.3322	0.9999	-1.1137	-2.5246	37.4201	-39.3944	0.1966	-1.6249	268.7225	414.8760	0.9526

10.4029	1.6181	3.4431	-4.2850	5.0337	0.9999	-1.0328	-2.7914	35.2602	-37.0496	-0.0654	-1.0201	-204.7235	224.0477	0.9974
	1.6001	3.4736	-4.2991	5.0419	0.9999	-1.0468	-2.7461	35.6566	-37.6070	-0.0364	-1.1124	-210.3732	-6607.4544	0.9962
	1.5908	3.5008	-4.3427	5.0753	0.9999	-1.0590	-2.7064	35.9938	-38.0826	0.0136	-1.2263	217.9978	1196.3393	0.9939
	1.5887	3.5765	-4.3434	5.0714	0.9999	-1.0645	-2.6894	36.1995	-38.5652	0.0787	-1.3864	-222.0644	-110.6573	0.9912
	1.5932	3.5996	4.4042	-5.1170	0.9999	-1.0741	-2.6583	36.4516	-38.9114	0.1219	-1.4755	-227.7626	256.6154	0.9871
	1.6026	3.6867	-4.4398	5.1424	0.9999	-1.0804	-2.6373	36.6513	-39.1868	0.1797	-1.5882	-235.5000	-1533.6323	0.9820
	1.6170	3.7737	4.4782	-5.1683	0.9999	-1.0896	-2.6066	36.8923	-39.3763	0.2061	-1.6399	-243.5619	-1164.1510	0.9746
	1.6354	3.8596	-4.5235	5.1989	0.9999	-1.0998	-2.5719	37.1253	-39.4633	0.2305	-1.6720	-253.6250	-7272.6522	0.9670
	1.6606	3.9596	-4.5793	5.2384	0.9999	-1.1109	-2.5344	37.3707	-39.4893	0.2306	-1.6682	264.4829	-299.2640	0.9562

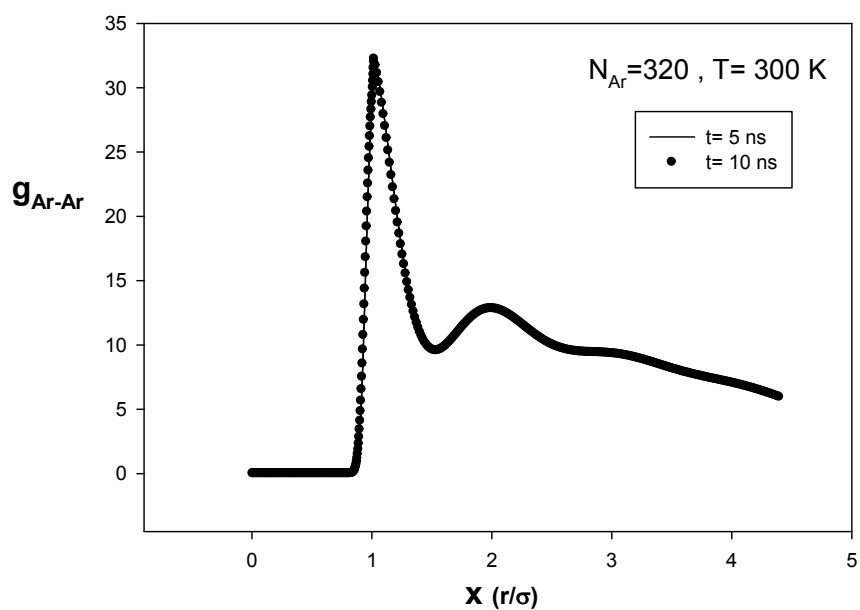
## 2- Testing the equilibration

In order to find the proper equilibration time in which the maximum number of the argon atoms enter to the nanotube can be obtained, one (33,0) CNT was immersed in an equilibrated periodic LJ fluid reservoir containing 8000 argon atoms. Without any filling, an initial optimization at the pressure of 1 atm and the temperature of 300 K was performed and the argon atoms were allowed to fill into the nanopore from the bulk outer fluid for 1, 3, 5, 7, and 10 ns. After completing the filing process, we determined the number of the confined atoms and presented them in the Fig. S2:



**Fig. S2.** The number of the confined atoms into the (33,0) CNT at different equilibration times

According to Fig. S2, after 5 ns, the number of the confined atoms do not change. Therefore, the equilibration time of 5 ns is the optimum (by considering the smallest computational cost). We have also compared the Ar-Ar RDF of the confined atoms at two equilibration times of 5 and 10 ns in Fig. S3:



**Fig. S3.** Comparison between the Ar-Ar RDF of the confined atoms at two equilibration times of 5 and 10 ns.

According to Fig. S2, the RDF values at the time larger than the equilibrium (10 ns) are the same as those results at the equilibration time (5 ns). Therefore, the 5 ns is the optimum time for the equilibration step.