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

ELECTRONIC SUPPLEMENTARY INFORMATION (ESI) for Model Atomistic Protrusions Favouring Ordering and Retention of Water

Prithvi Raj Pandey* and Sudip Roy

Physical Chemistry Division,

National Chemical Laboratory,

Pune-411008, India.

Tel. No. - +91 (020) 25903148, Fax No. - +91 (020) 25902636

Email: pr.pandey@ncl.res.in

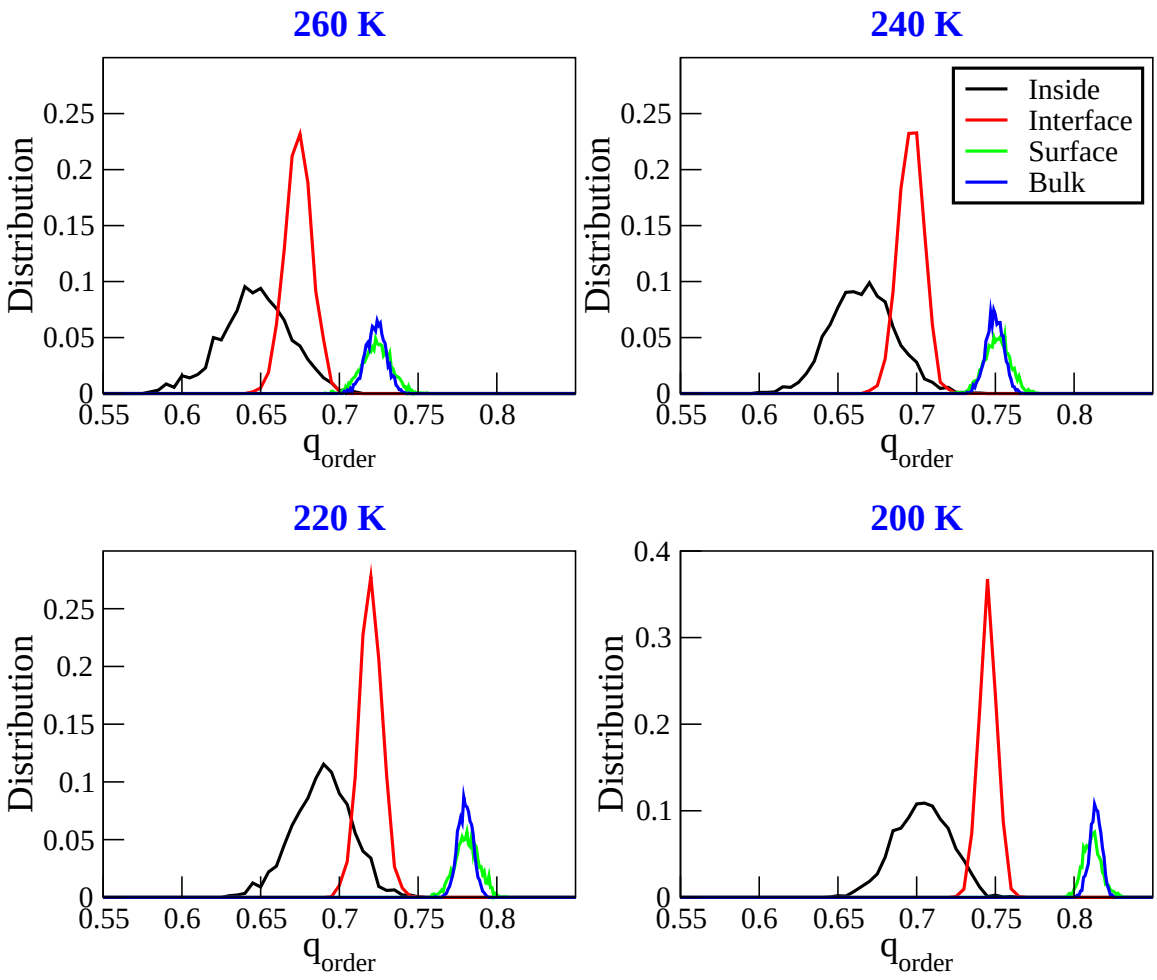

Figure 1: Distribution of q_{order} at 1 bar and different temperature. It indicates that at a particular temperature and pressure the value of q_{order} varies as inside <interface <surface $\simeq$ bulk.

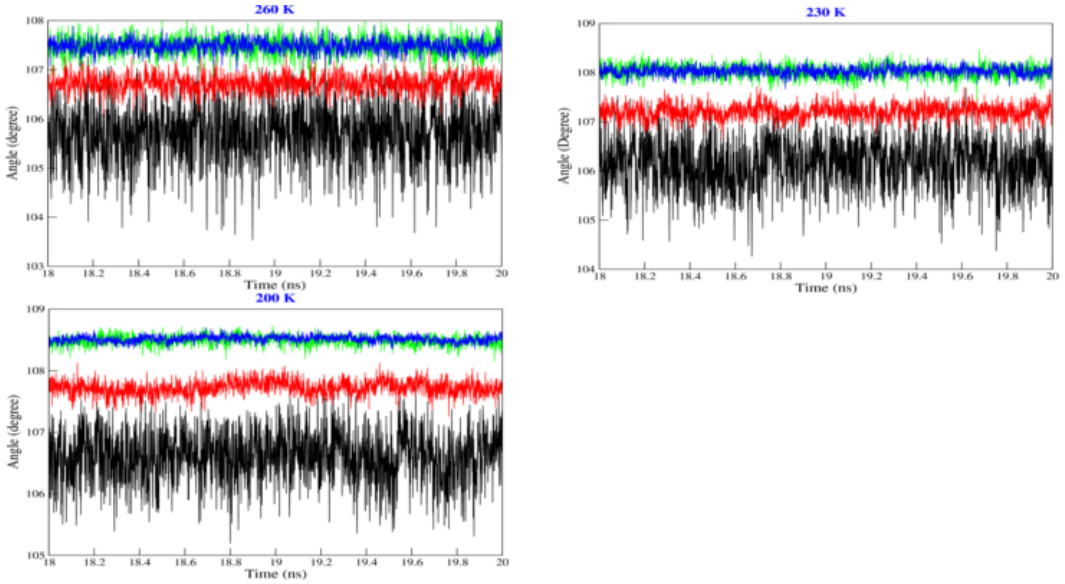

Figure 2: θ_{ij} in q_{order} as a funtion of time for different temperatures and 1 bar pressure.

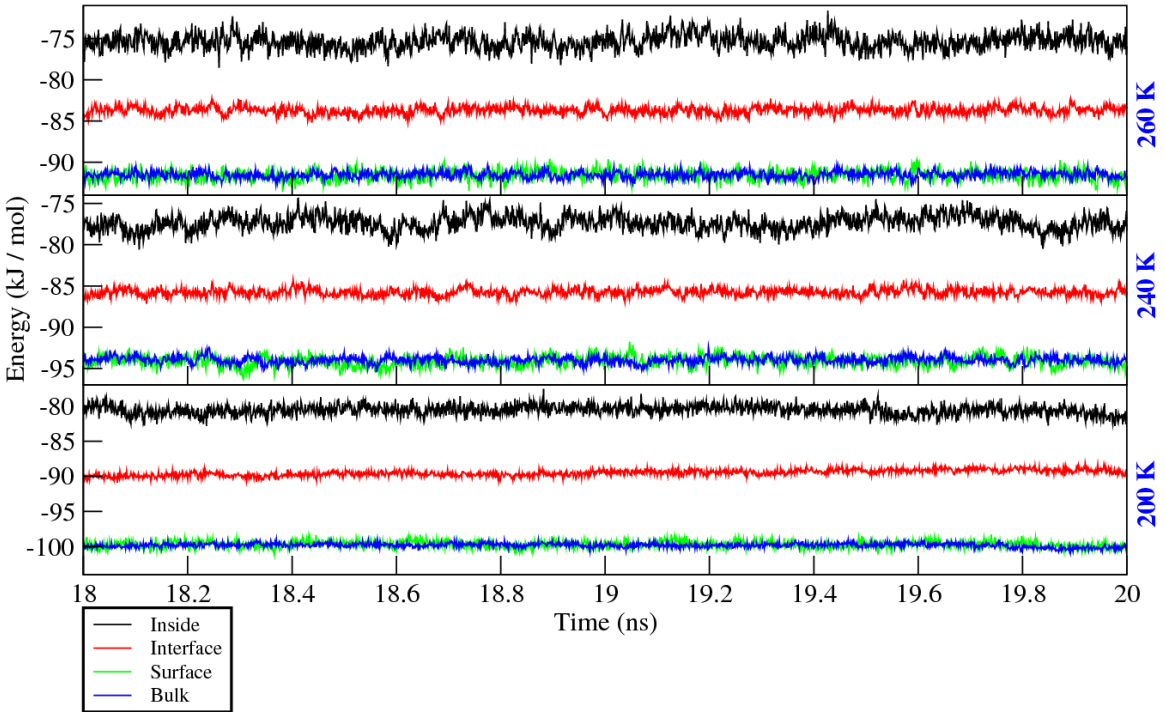

Figure 3: Plot of average nonbonded potential energy per water molecule as a function of time for different temperatures and 1 bar pressure.

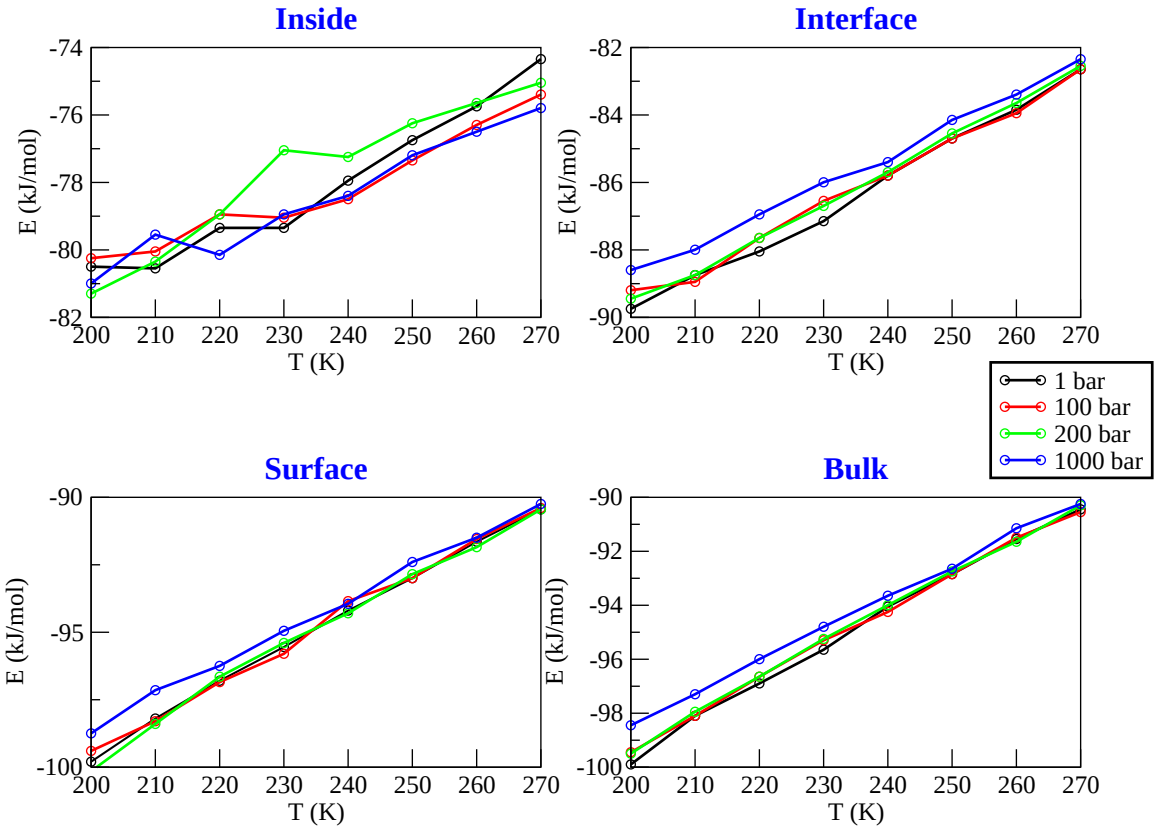

Figure 4: Peak height of potential energy distribution as a function of temperature at different pressures.

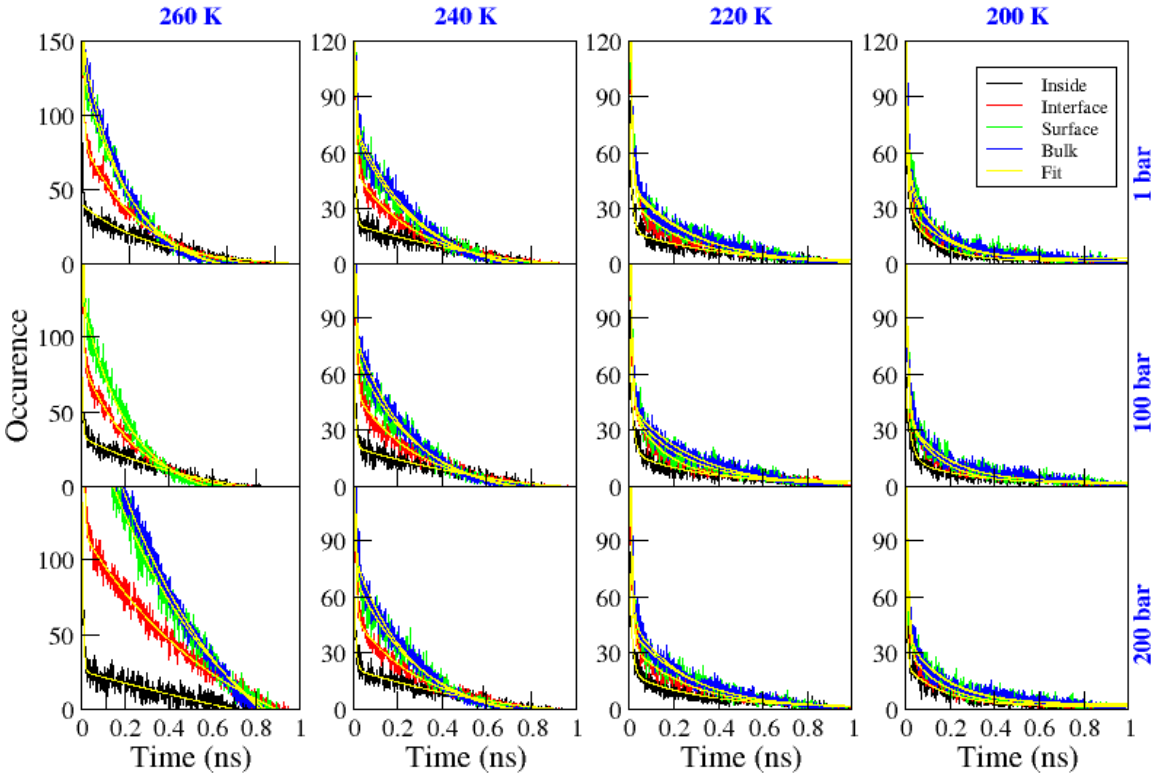

Figure 5: Fitting of of residence time with bi-exponential function.

Table 1: Components of bi-exponential fitting of residence time distribution at different temperatures and pressures.

	Inside				Interface				
260K	a_s	τ_s **(ns)**	a_s	τ_s**(ns)**	**260K**	a_s	τ_s **(ns)**	a_s	τ_s**(ns)**
1 bar	45.5469	0.5736	91.6534	0.004318	**1 bar**	89.4762	0.2385	225.464	0.005286
100 bar	45.3208	0.573	85.588	0.004546	**100 bar**	89.1516	0.2360	226.788	0.005337
200 bar	103.621	2.478	222.344	0.005158	**200 bar**	162.071	0.6702	418.232	0.006191
240K					**240K**				
1 bar	36.1919	0.9703	84.6565	0.007076	**1 bar**	52.4022	0.2791	192.458	0.007444
100 bar	33.962	0.9169	77.9956	0.007141	**100 bar**	53.3352	0.2705	184.014	0.007580
200 bar	33.2244	0.8365	78.5308	0.007506	**200 bar**	52.1139	0.2938	178.069	0.00720
220K					**220K**				
1 bar	18.6233	0.5007	61.7121	0.01247	**1 bar**	33.483	0.2394	163.719	0.009469
100 bar	16.9514	0.3560	64.9655	0.01443	**100 bar**	38.1451	0.1719	150.357	0.008678
200 bar	17.3841	0.3603	56.745	0.01369	**200 bar**	34.0236	0.2490	141	0.00928
200K					**200K**				
1 bar	28.5703	0.1240	81.3607	0.007949	**1 bar**	30.5753	0.1865	112.991	0.009711
100 bar	13.6863	0.2501	42.2989	0.02141	**100 bar**	36.8842	0.1423	118.033	0.00824
200 bar	21.8807	0.1745	77.3748	0.005857	**200 bar**	30.5296	0.1674	110.773	0.009760

	Surface				Bulk				
260K	a_s	τ_s **(ns)**	a_s	τ_s**(ns)**	**260K**	a_s	τ_s **(ns)**	a_s	τ_s**(ns)**
1 bar	140.074	0.2062	283.761	0.003798	**1 bar**	155.676	0.1814	284.609	0.003581
100 bar	135.374	0.2166	272.392	0.004393	**100 bar**	153.632	0.1867	276.208	0.003420
200 bar	272.698	0.5634	512.935	0.004305	**200 bar**	307.295	0.5681	495.405	0.004230
240K					**240K**				
1 bar	77.8862	0.2712	213.621	0.00582	**1 bar**	83.4287	0.2871	252.992	0.005916
100 bar	77.8739	0.2811	230.353	0.006424	**100 bar**	87.8087	0.2508	226.523	0.006104
200 bar	78.5998	0.2927	238.374	0.005538	**200 bar**	88.347	0.2582	251.074	0.005069
220K					**220K**				
1 bar	42.3192	0.2620	190.485	0.007690	**1 bar**	43.5488	0.2756	193.799	0.008254
100 bar	39.636	0.2371	162.412	0.009729	**100 bar**	44.5122	0.2838	196.185	0.00811
200 bar	42.8219	0.285	194.775	0.007021	**200 bar**	47.8152	0.2464	170.044	0.008678
200K					**200K**				
1 bar	51.3495	0.1148	130.027	0.006577	**1 bar**	42.2377	0.1468	133.635	0.008365
100 bar	34.6056	0.1830	122.683	0.01069	**100 bar**	35.2742	0.1850	122.917	0.01055
200 bar	36.2709	0.1789	118.605	0.009263	**200 bar**	35.6283	0.1867	155.314	0.009083