Supplementary Material

Water-Ice III Interfacial Free Energy: A Mold Integration study using the TIP4P/Ice model.

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Table 1: $\bar{q}_6$ threshold as a function of pressure.

Pressure (bar)	r_c (Å)	$\bar{q}_{6,t}$	% mislabel
1400	5.0	0.0755	2.28
3000	5.0	0.0751	2.26
5000	5.1	0.0694	1.44
7000	5.0	0.0754	1.6

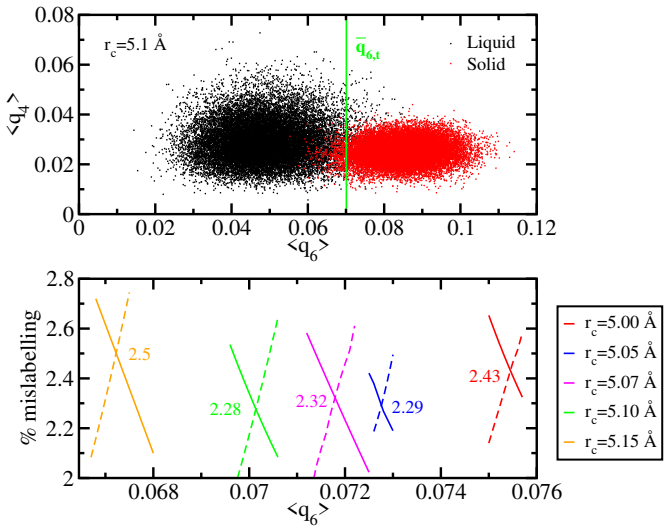

Figure 1: top: Lechner and Dellago order parameters q_4 and q_6 for solid (ice III) and liquid water using the TIP4P/Ice water model as indicated in the legend at 1400 bar and 256.5 K. bottom: mislabeling in the liquid and the solid using different cut-off radii.

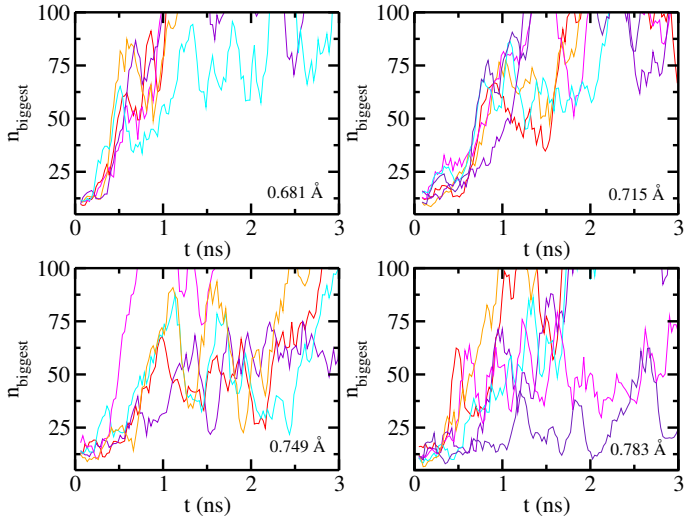

Figure 2: Number of water molecules of the biggest cluster *vs* time for several trajectories and different well radii (as indicated in the legend) for the 001 plane of wells exposed at the interface at 1400 bar at the melting point.

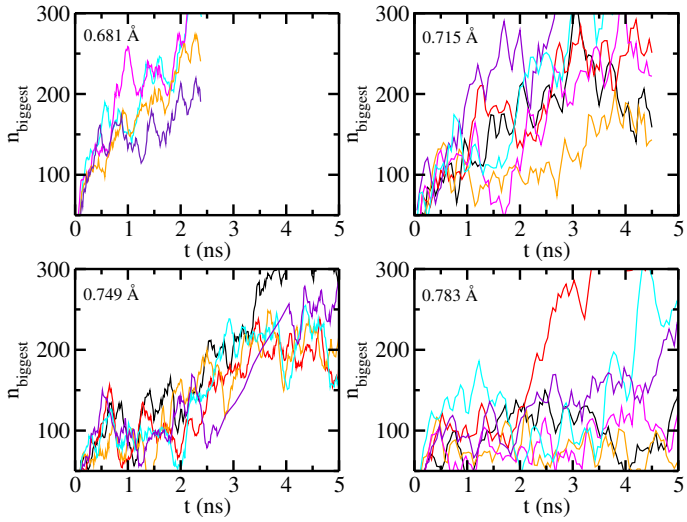

Figure 3: Number of water molecules of the biggest cluster *vs* time for several trajectories and different well radii (as indicated in the legend) for the 100 plane of wells exposed at the interface at 3000 bar at the melting point.

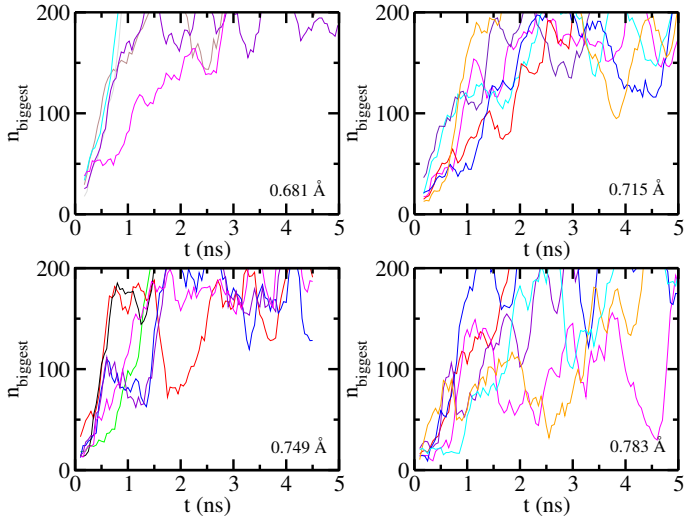

Figure 4: Number of water molecules of the biggest cluster *vs* time for several trajectories and different well radii (as indicated in the legend) for the 001 plane of wells exposed at the interface at 5000 bar at the melting point.

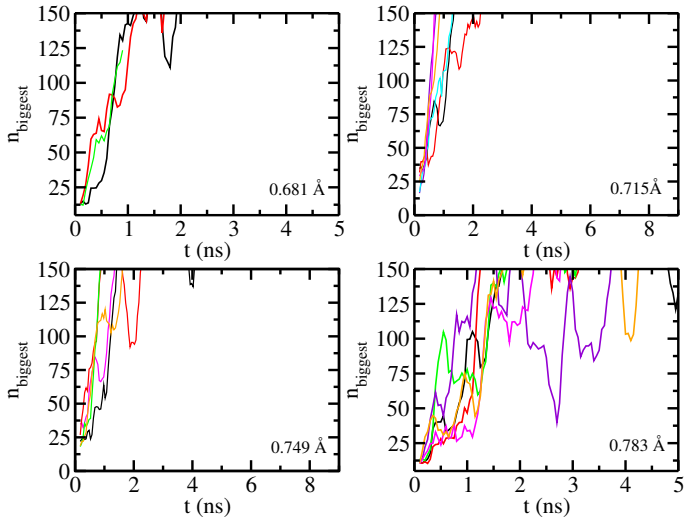

Figure 5: Number of water molecules of the biggest cluster *vs* time for several trajectories and different well radii (as indicated in the legend) for the 001 plane of wells exposed at the interface at 7000 bar at the melting point.

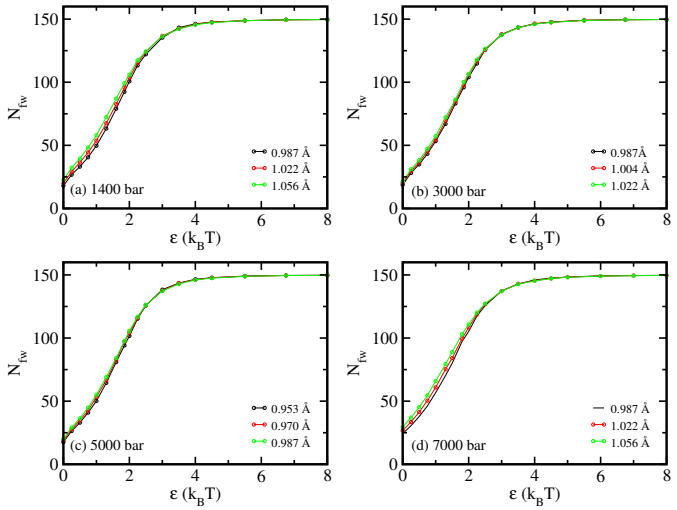

Figure 6: Number of filled wells as a function of the potential interaction (ε) for values $r_w > r_w^o$ of the 001 plane of ice III using the TIP4P/Ice water potential for different isobars.