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


# Supplementary Information

## Why the cubic structure of ice is preferred in the newly formed ice?

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Simulation procedure for the simulations of pure liquid water

Computer simulations were conducted with the use of Amber12[1] molecular dynamics package and TIP4P-Ice[2] water model. A simulation system consisted of 12 665 molecules of liquid water located in a rectangular simulation box. A preliminary equilibration was performed in NpT conditions for 2 ns at temperature of 300 K. The temperature was kept constant by the weak coupling to an external bath ($\tau_T$ = 1.0 ps) using the Berendsen thermostat[3]. The pressure (1 bar) was kept constant by the weak coupling method ($\tau_P$ = 1.0 ps). The particle-mesh Ewald method was used for electrostatic interactions and the length of chemical bonds involved hydrogen atoms were fixed with the use of SHAKE algorithm. A cutoff of 1.2 nm for nonbonding interactions was used. After the equilibration, the final simulations were performed at each of the selected temperature (within the range 250 – 300 K). The lengths of the obtained trajectories were equal to 2.4 ns.


1 D. A. Case, T. A. Darden, T. E. Cheatham III, C. L. Simmerling, J. Wang, R. E. Duke, R. Luo, R. C. Walker, W. Zhang, K. M. Merz, B. Roberts, S. Hayik, A. Roitber, G. Seabra, J. Swails, A. W. Götz, I. Kolossváry, K. F. Wong, F. Paesani, J. Vanicek, R. M. Wolf, J. Liu, X. Wu, S. R. Brozell, T. Steinbrecher, H. Gohlke, Q. Cai, X. Ye, J. Wang, M.-J. Hsieh, G. Cui, D. R. Roe, D. H. Mathews, M. G. Seetin, R. Salomon-Ferrer, C. Sagui, V. Babin, T. Luchko, S. Gusarov, A. Kovalenko and P. A. Kollman, *Amber 12. Reference Manual*, University of California, San Francisco, 2012.

2 J. L. F. Abascal, E. Sanz, R. García Fernández and C. Vega, A potential model for the study of ices and amorphous water: TIP4P/Ice, *J. Chem. Phys.*, 2005, **122**, 234511.

3 H. J. C. Berendsen, J. P. M. Postma, W. F. van Gunsteren, A. DiNola and J. R. Haak, Molecular dynamics with coupling to an external bath, *J. Chem. Phys.*, 1984, **81**, 3684–3690.

Figure S1

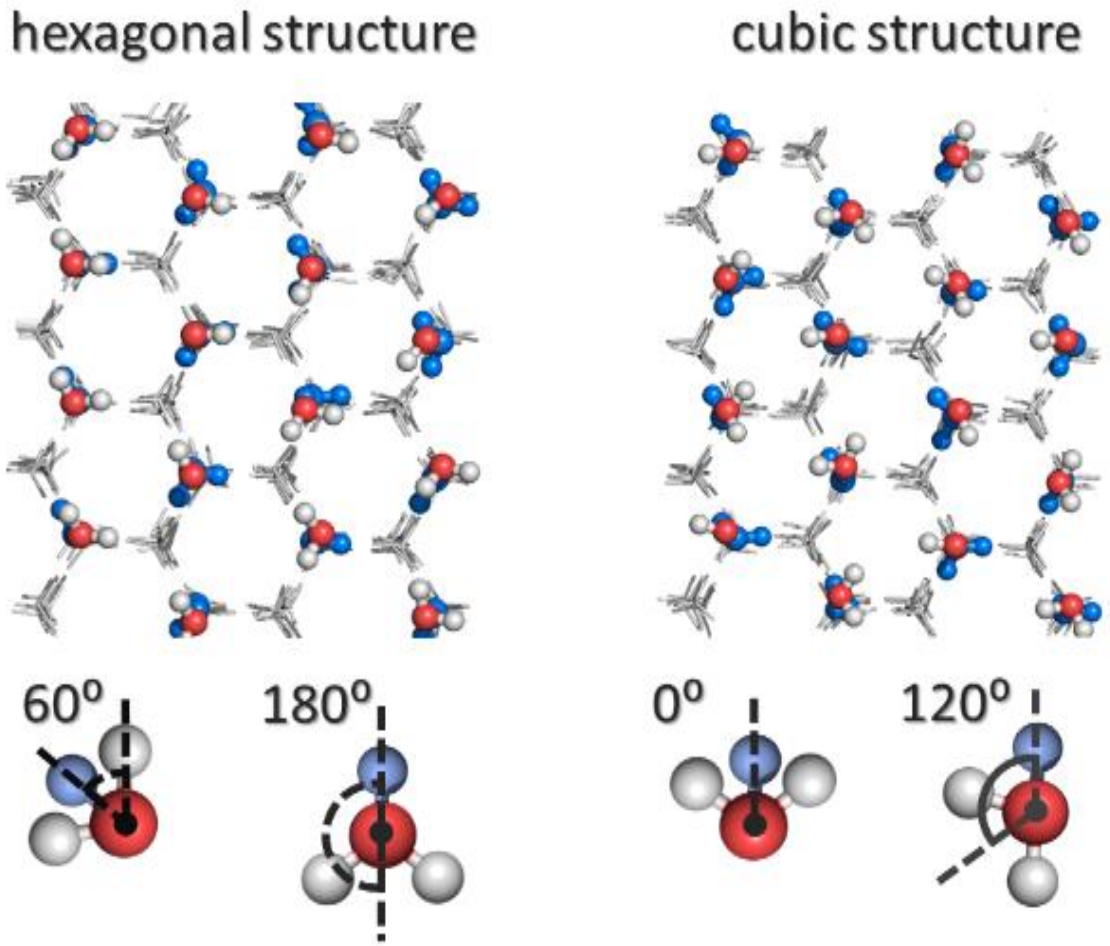


*Figure S1. Relative orientations of water molecules that form hydrogen-bonded pairs and are located within the adjacent layers of emerging ice. The figure illustrates the state of the systems consisted of the crystal of ice and liquid water simulated at 250 K, after 18 ns of simulation. The molecules marked in white and red are located within the newly formed layer of ice, while the molecules marked as blue are located directly beneath them and are a part of the original crystal of ice. The crystal lattice of the hexagonal ice (marked in grey) has been shown for reference. The figure was generated with the use of PyMOL* [1]

1 Schrödinger, The PyMOL Molecular Graphics System, version 2.1, *LCC*.

Table S1

| Temperature [K] | $p_{hex}$ | $p_{cub}$ | $p_{cub}/p_{hex}$ |
|---|---|---|---|
| 250 | 0.1440 | 0.1856 | 1.2889 |
| 260 | 0.1472 | 0.1820 | 1.2365 |
| 265 | 0.1486 | 0.1806 | 1.2159 |
| 270 | 0.1494 | 0.1799 | 1.2040 |
| 280 | 0.1513 | 0.1777 | 1.1744 |
| 290 | 0.1529 | 0.1761 | 1.1512 |
| 300 | 0.1539 | 0.1752 | 1.1385 |

*Table S1. The probabilities for a pair of molecules in liquid water to adopt a relative orientation characteristic for hexagonal ($p_{hex}$) and cubic ($p_{cub}$) structure of ice calculated for temperatures in range of 250 - 300 K.*