# Can we call the transition between low-density and high-density amorphous ices as a first-order transition?

**Shupletsova A A**[1,2,@] **and Stegailov V V**[1,2,3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[@] garkul.aa@phystech.edu

Water polymorphism has been extensively studied, but there is still controversy over the phase transition between high-density amorphous ice (HDA) and low-density amorphous ice (LDA). And computer modelling plays an important role in understanding the relationships between different states of water.
In this paper, we report a molecular dynamics study of pressure-induced LDA-HDA transitions using the TIP4P/Ice water model. Our algorithm for identifying clusters of one structure within another is based on differences in intermediate range order [1]. The presented picture of nucleation makes it possible to visually estimate the size of "critical nuclei" and compare the result with experiment [2]. At the next stage of the transition, nucleation growth phenomena are observed. Finally, the dependence of the position of the kinetic spinodal on the compression rate is discussed. The result is compared with the experimental data [3], and also with the assumed position of the second critical point of water [4].

[1] Garkul A and Stegailov V 2022 *Scientific Reports* **12** 13325
[2] Tonauer C M, Seidl-Nigsch M and Loerting T 2017 *Journal of Physics: Condensed Matter* **30** 034002
[3] Gromnitskaya E, Stal'gorova O, Brazhkin V and Lyapin A 2001 *Physical Review B* **64** 094205
[4] Debenedetti P G, Sciortino F and Zerze G H 2020 *Science* **369** 289–292