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Hypothetical Ultralow-density Ice Polymorphs

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Among 17 known ice polymorphs, only two are less dense than normal ice, and they are made very recently by a tricky procedure, vacuum pumping the small guest molecules from clathrate hydrate. The discovery of low-density ice polymorphs opens the door to the survey on ices under negative pressures. Negative pressure is very hard to be accessed experimentally, and theoretical predictions are indispensable. How many stable phases are possible for ices under negative pressures? Are two ices really the most stable phases at some thermodynamic conditions? How low can the density of ice be? Exhaustive evaluation of sparse ice structures and theoretical considerations provide unexpected answers to these questions.

Significance statement

This is the first exhaustive survey on the low-density ice polymorphs. We found a couple of more stable zeolitic ices ever, and also a family of many possible low-density structures named “aeroices”.

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Track Classification: Ice Crystal Growth