Geophysical Research Abstracts
Vol. 20, EGU2018-18282-1, 2018
EGU General Assembly 2018

Understanding homogeneous ice nucleation with computer simulations

Eduardo Sanz and Jorge Espinosa
Physical Chemistry Department, UCM, Madrid, Spain

In the last 5 years we have been using computer simulations
with the aim of shedding light in the process of ice nucleation.
Such process is the first step of water freezing, arguably the liquid-to-solid
transition with the greatest relevance on Earth. In particular, the
extent of freezing in atmospheric clouds has a great impact on the
Earth's albedo and, therefore, on climate change.
Simulations is a particularly suitable tool to study ice nucleation
because it enables access to the time and length scales
relevant to this process, ns and nm, complementing the
information obtained in experiments where such small
scales can not be probed.

Using simple models for simulating water we have been
able to reach a fairly good agreement with experimental
ice nucleation rates [1]. We have used the information drawn in
our simulations to gain a better understanding of the
ice nucleation process in terms of molecular mechanism and thermodynamic
parameters affecting the nucleation rate. With this information
we propose a tentative explanation for the decelerating effect
of pressure on ice nucleation [2,3] as well as for current discrepancies
in measurements of the nucleation rate between different experimental groups [4].
By comparing ice nucleation under pressure and in a brine solution we
have also examined [5] the proposal that ice nucleation can be predicted in terms
of water activity [6].

[1] E. Sanz, C. Vega, J. R. Espinosa, R. Caballero-Bernal,
J. L. F. Abascal, and C. Valeriani,
"Homogeneous ice nucleation at moderate supercooling from molecular simulation,"
JACS, vol. 135, no. 40, pp. 15008–15017, 2013.

[2] H. Kanno, R. J. Speedy, and C. A. Angell,
"Supercooling of water to -92 C under pressure,"
Science, vol. 189, no. 4206, pp. 880–881, 1975

[3] J. R. Espinosa, A. Zaragoza, P. Rosales-Pelaez,
C. Navarro, C. Valeriani, C. Vega, and E. Sanz,
"Interfacial free energy as the key to the pressure-induced deceleration of ice nucleation,"
Phys. Rev. Lett., vol. 117, p. 135702, 2016

[4] Espinosa, J. R.; Navarro, C.; Sanz, E.; Valeriani, C.; Vega, C.
"On the time required to freeze water"
J. Chem. Phys., vol. 145, 211922, 2016

[5] J. R. Espinosa, G. D. Soria, J. Ramirez, C. Valeriani,
C. Vega, and E. Sanz,
"Role of salt, pressure, and water activity on homogeneous ice nucleation,"

J. Phys. Chem. Lett., vol. 8, p. 4486, 2017

[6] T. Koop, B. Luo, A. Tsias, and T. Peter,
"Water activity as the determinant for homogeneous ice nucleation in aqueous solutions,"
Nature, vol. 406, pp. 611–614, 2000