Studying NaCl crystal nucleation from aqueous solutions

C. P. Lamas[1,2], J. R. Espinosa[3], M. M. Conde[4], J. Ramírez[4], P. Montero de Hijes[1], E. G. Noya[2], C. Vega[1], and E. Sanz[1]

[1]Departamento de Química Física (Unidad de I+D+i asociada al CSIC)

[2]Instituto de Química Física Rocasolano, Consejo Superior de Investigaciones Científicas, CSIC, Calle Serrano 119, 28006 Madrid, Spain

[3] Maxwell Centre, Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge CB3 0H3, United Kingdom

[4] Departamento de Ingeniería Química Industrial y Medio Ambiente, Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid, 28006, Madrid, Spain

The Seeding method is an approximate approach to investigate nucleation that combines molecular dynamics simulations with classical nucleation theory. This technique has been successfully implemented in a broad range of nucleation studies in the recent years. However, its accuracy is subject to the arbitrary choice of the order parameter threshold used to distinguish liquid-like from solid-like molecules [2]. We revisit here the crystallisation of NaCl from a supersaturated brine solution and show that consistency between Seeding [1] and rigorous methods like Forward Flux Sampling [3] or spontaneous crystallisation [1, 3, 4], is achieved by following a mislabelling criterion to select such threshold (i. e. equalling the fraction of mislabelled particles in the bulk parent and nucleating phases) [5]. This work supports the use of Seeding to obtain fast and reasonably accurate nucleation rate estimates and the mislabelling criterion as one giving the relevant cluster size for classical nucleation theory in crystallisation studies (see Fig. 1).

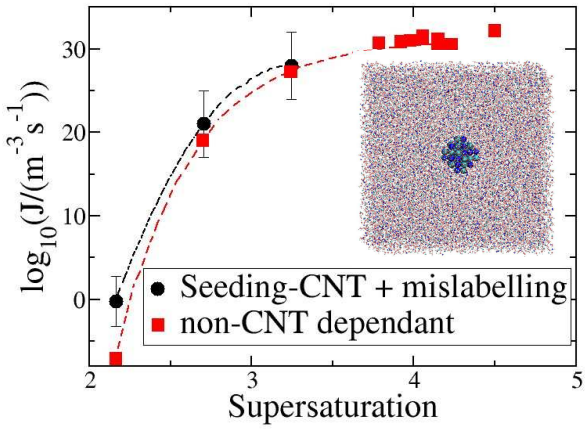

Fig. 1. Decimal logarithm of the nucleation rate vs. supersaturation, obtained with the seeding technique and mislabelling criterion (black circles)[1], and with non classical nucleation theory methods (red squares) [1, 3, 4].

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