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Computer Simulations of Ice Growth from Pure and Salty Water MARCELO CARIGNANO, IGAL SZLEIFER, Purdue University — A six-site water model recently proposed by H. Nada et al (J. Chem. Phys. 118, p7401, 2003) is extensively studied in relation to its ability to reproduce the growing of a crystal phase over the supercooled liquid. We perform Molecular Dynamics simulations at constant pressure and several temperatures below and above the melting temperature of the model, and the resulting kinetics is analyzed in terms of classical nucleation theory. The effect of adding dissociated sodium chloride on the kinetics of crystallization and the structure of water-ice interface is also studied. Preliminary results show that upon crystallization the ions occupy lattice position replacing Oxygen, and in all cases studied so far the ions are found in pairs.

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