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Physics of solid and liquid alkali halide surfaces near the melting point TATYANA ZYKOVA-TIMAN, DAVIDE CERESOLI, UGO TARTAGLINO, SISSA, INFM, Democritos, via Beirut 2-4, ERIO TOSATTI, SISSA, Democritos, ICTP, P.O. Box 586, I-34014 Trieste, Italy — NaCl (and other alkali halide) crystal surfaces have the peculiar property of repelling their own melt. As a result they let themselves be wetted only partially by their own liquid at the melting point T_M. We recently investigated the physical reasons for this unusual behavior. We found them through theory and molecular dynamics simulation to stem from the conspiracy of three factors. First, the solid NaCl(100) surface is exceptionally anharmonic,but also exceptionally stable. It can in fact survive even well above the melting point, for unlike most other surfaces it does not spontaneously melt. Second, the solid-liquid interface is very costly, due to a 27% density difference between solid and liquid. Third, the surface tension of liquid NaCl is relatively high. This last feature is due to an unexpected entropy deficit, that can in turn be traced to incipient molecular charge order in the outermost regions of the molten salt surface[1,2].
[1] T. Zykova-Timan, D. Ceresoli, U. Tartaglino, E. Tosatti, Phys. Rev. Lett. 94, 176105 (2005)
[2] T. Zykova-Timan, D. Ceresoli, U. Tartaglino, E. Tosatti, J. Chem. Phys. 123, 164701 (2005)

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