

Water-Triggered Conduction and Polarization Effects in a Hygroscopic Fullerene Salt

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Impedance spectroscopy is employed to probe the frequency-dependent conductivity and dielectric response of the crystalline $C_{60}O_{24}Na_{24}$ fulleride, both in its pure form obtained by heating to 473 K and in its bulk-hydrate form stable only below 390 K, of chemical formula $C_{60}O_{24}Na_{24} \cdot 16 H_2O$. A dielectric loss feature is visible in both the pure material and the hydrate, displaying different strength and activated behavior in different temperature ranges.

Charge conduction in the pure material is mainly electronic in the whole temperature range studied. Exposure of the pure material to humid atmosphere results in an increase of the room-temperature conductivity by four orders of magnitude due to hydration of the surface of the crystalline grains, a situation encountered in many other systems.[1]. The surface water is desorbed by annealing to 330 K.

The conductivity of the hydrate is dominated between 320 and 390 K by a water-related contribution, possibly due to proton shuttling. Due to such contribution, at 360 K the conductivity of the hydrate is higher than that of the pure material by almost two orders of magnitude.

The relaxation feature in the pure material is found to have a conductivity origin (conductivity-induced dielectric loss [2]), but its frequency and intensity are affected by the presence of water. The hydrate material contains both structural bulk water and surface hydration water. The bulk water does not lead to any relaxation feature, in agreement with the expectation for a crystalline hydrate with an important hydrogen-bond network. The presence of surface water leads instead to the appearance of an intense dipolar loss feature in the radiofrequency region, which shows a non-monotonic temperature dependence similar to other water-containing systems. [3]

[1] H. Haspel et al., J. Phys. Chem. C 2013, 117, 16686–16697

[2] S. Capaccioli et al., J. Phys.: Cond. Matter 1998, 10, 5595–5617

[3] R. Macovez et al. J. Phys. Chem. C 2014, 118 (9), 4941–4950