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Surface-trapped excess electrons on ice FRANCESCA BALETTO, MAL-SOON LEE[1], SANDRO SCAMDOLO, The Abdus Salam ICTP and INFM-CNR Democritos, Trieste (Italy) — Local surface trapping of excess electrons has recently been observed in large water clusters and at the ice/vacuum interface. The existence of stable surface-bound states for the excess electron may have important implications in atmospheric chemistry, electrochemistry, and radiation physics. By means of first-principles molecular dynamics we find that excess electrons induce a structural reconstruction of the ice surface on a time scale of a fraction of a picosecond [Baletto et al., PRL 95, 176801 (2005)]. Preliminary results on small neutral water clusters indicate that fast (on a picoseconds scale) structural changes occur already at the lowest atmospheric temperatures, suggesting that addition of excess electrons may lead to even more substantial structural rearrangements than those found for the ice surface.

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