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Material simulation of charge carrier transport properties of polymer dielectrics MIKAEL UNGE, ABB Corporate Research SE 72178 Vsters, Sweden, THOMAS CHRISTEN, ABB Corporate Research Baden-Dttwil, Switzerland, CHRISTER TRNKVIST, ABB Corporate Research SE 72178 Vsters, Sweden, ABB CORPORATE RESEARCH TEAM — To understand electron and hole transport in solid material requires to know its electronic properties, i.e. the density of states (DOS) and whether the states are spatially localized or delocalized. The states closest to the band edges may be localized, states further away can be delocalized. This transition from localized to delocalized states determines the mobility edge, above the mobility edge the mobility is expected to be high. A real polymer is never perfect; it contains a number of oxidative states, bonding defects and molecular impurities. These imperfections yield electronic states that can appear in the band gap of the polymer, traps. Traps can be shallow, i.e. close to the band edges, from these states the charge carrier easily can jump to a state in the band edge or another shallow state. Other traps can be deep, in these states it is likely that the charge carrier remains and become immobile. All these properties related to the electronic structure of the polymer, including its defects, affects the conductivity of the polymer. Linear scaling Density Functional Theory has been applied to calculate electronic structure of amorphous polyethylene. In particular DOS, trap levels and mobility edges are studied.

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