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Model *ab initio* studies of solvation and excess charge localization on conjugated carbon chains[1] MICHAEL MAYO, YURI GARTSTEIN, The University of Texas at Dallas — Using long C_NH_2 conjugated carbon chains with the polyynic structure as prototypical examples of one-dimensional (1D) semiconductors, we discuss self-localization of excess charge carriers in the presence of the interaction with a surrounding polar solvent. The solvation mechanism of self-trapping is different from the self-localization due to coupling with bond-length modulations of the underlying atomic lattice well-known in conjugated polymers. Model *ab initio* computations are carried out and compared that employ various methods such as hybrid density functionals and Hartree-Fock within the framework of the polarizable continuum model. We demonstrate the possibility of the formation of large 1D electron- and hole-polarons entirely due to solvation, but even larger degrees of charge localization occur when accompanied by atomic displacements. Also discussed are doubly-charged bipolaron states and topological kink-solitons that may be formed in these systems. For a brief report, see M. L. Mayo and Yu. N. Gartstein, Phys. Rev. B 78, 073402 (2008).

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