

Abstract Submitted
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Charge carrier solvation on a polymer chain revealed in *ab initio* computations¹ MICHAEL MAYO, YURI GARTSTEIN, The University of Texas at Dallas, Richardson, Texas, USA — When an excess charge carrier (electron or hole) is added to a semiconducting polymer chain in vacuum, it is well known that the carrier may self-trap into a polaronic state accompanied by a self-consistent localized bond alternation pattern. A different mechanism of self-localization is a solvation of the charge carrier expected to take place when the polymer chain is immersed in a polar medium (such as a common solvents) - in this case a self-consistent pattern of the orientational polarization is formed around a localized charge. The goal of our study is to identify this solvation effect within *ab initio* computations. Using long carbon atom chains (both hydrogen terminated and rings) as model systems, we employ the hybrid B3LYP density functional within the DFT and the Polarizable Continuum Model to find the resulting electronic level structure and atomic charge densities. Our results clearly show trends towards excess charge self-localization due to the solvation. We suggest that this effect may be of importance for various semiconductor nanostructures in polar environments.

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