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Soliton and polaron induced 3D conformational changes in conjugated polymers[1] ANDRE LEITAO BOTELHO, XI LIN[2], Boston University — We perform ab initio calculations on polyacetylene (PA), polypyrrole (PPY), and polyaniline (PANI) to examine the 3D conformational change as a function of injected charge. We find that self-localized solitons and polarons in their ground states are dispersed along the chain to minimize the localized charge Coulomb repulsion and the strain repulsion due to chain terminations. Each polaron in PPY or PANI progressively straightens each chain from their neutral bent state, where PPY and PANI are shown to have analogous conformations due to subsequent twisting along non-collinear axes. Solitons in PA are able to fully utilize the zigzag backbone geometry to minimize Coulomb repulsions, by alternating from one side of the chain to the other. This causes bending in alternating directions, leading to a sinusoidal shape, while maintaining a straight chain axis on average. Since PPY and PANI can change from a coil to a straight rod, these polymers can achieve strains about an order of magnitude higher than PA.

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