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Estimating the electronic conductivity of size-expanded DNA: a complex bandstructure study MIGUEL FUENTES-CABRERA, JACK C. WELLS, Oak Ridge National Laboratory, OSCAR HUERTAS, F. JAVIER LUQUE, Facultat de Farmacia, Universitat de Barcelona, HAO WANG, JAMES P. LEWIS, Department of Physics and Astronomy, Brigham Young University, MODESTO OROZCO, Institut de Recerca Biomedica and Facultat de Quimica, Universitat de Barcelona, OTTO F. SANKEY, Department of Physics and Astronomy, Arizona State University — xDNA is a new class of synthetic nucleic acid with one of the bases larger than the natural congeners. The larger bases, called x-bases, can be viewed as a synthesis of benzene and a natural base. We recently have found that the x-bases have HOMO- LUMO gaps smaller than their natural congeners, and that size- expanded duplexes have stronger π-π stacking interactions than B-DNA duplexes. These findings suggest that xDNA is likely to have a smaller band gap than B-DNA, which could make xDNA a candidate for molecular wire applications. Here we use the complex band-structure method to estimate the conductive properties of polyxG.polyC and polyxG.polyxC. These results are compared to those we obtained previously on polyG.polyC. In this manner, we systematically probe how changes in the π-π stacking interactions affect the conductivity of DNA-like molecules.

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