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Density Functional Theory Study of Polyanilines and Polypyrroles MONICA BASTOLA, SUDIP NEUPANE, PEDRO DEROSA, Louisiana Tech University — From the moment polymers were found to be able to conduct electricity, upon appropriate doping, a number of technological applications have been implemented and a large number of other applications are envisioned. There is however still a lack of deep understanding of the correlation between the properties at the molecular level and the corresponding properties at the macroscopic level. Bridging the gap, the development of a multiscale model able to connect the two words, is certainly a task that must be accomplished. One step towards that aim consists on the development of strategies that allow to infer from molecular properties macroscopic properties what requires sufficiently accurate and computationally inexpensive models able to study the evolution of molecular properties into macroscopic properties. This work presents a density functional study of polyanilines and polypyrroles, geometry, HOMO-LUMO gap energy, charge distribution and the molecular orbital structures are calculated as function of polymer size and structure. For the polypyrroles the relation between these properties and the oligomer size will be presented. For the polyanilines, the fully reduced leucoemeraldine based, the half oxidized emeraldine based and the fully oxidized pernigraniline are studied and compared.

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