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Porphyrin-based polymeric nanostructures for light harvesting applications: Ab initio calculations WALTER ORELLANA[1], Universidad Andres Bello — The capture and conversion of solar energy into electricity is one of the most important challenges to the sustainable development of mankind. Among the large variety of materials available for this purpose, porphyrins concentrate great attention due to their well-known absorption properties in the visible range. However, extended materials like polymers with similar absorption properties are highly desirable. In this work, we investigate the stability, electronic and optical properties of polymeric nanostructures based on free-base porphyrins and phthalocyanines (H_2P, H_2Pc), within the framework of the time-dependent density functional perturbation theory. The aim of this work is the stability, electronic, and optical characterization of polymeric sheets and nanotubes obtained from H_2P and H_2Pc monomers. Our results show that H_2P and H_2Pc sheets exhibit absorption bands between 350 and 400 nm, slightly different that the isolated molecules. However, the H_2P and H_2Pc nanotubes exhibit a wide absorption in the visible and near-UV range, with larger peaks at 600 and 700 nm, respectively, suggesting good characteristic for light harvesting. The stability and absorption properties of similar structures obtained from ZnP and ZnPc molecules is also discussed.

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