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Study of the dynamics of aggregation and behavior in the solution of substituted phthalocyanines

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Abstract: The study of electronic properties of photosensitizing compounds, in which the derivatives of porphyrins, phthalocyanines and naphthalocyanines are focused here, has attracted the interest of the academic community recently thanks to the wide range of applications as, e.g., in energy conversion for solar cells or in photodynamic therapy (PDT). [1,2] Using quantum methods to study part of this class of compoundswere carried out in order to obtain electronic properties, aiming their use as photosensitizers in PDT. For such application, electronic transition may occur in the region between 600 and 800 nm.[2,3] However, previous studies by our research group and other researchers emphasized the importance of understanding the aggregations of these compounds and their electronic implications. [4,5] Thus, this work proposes to study the dynamics of aggregation of Zn(II)-Phthalocyanines (ZnPc) and Zn(II)-Naflococyanines (ZnNc) and their tetrasubstituted variations with tert-butyls. As cells of the dynamics were modeled with approximately 4000 SPC water molecules using the GROMOS 53a6 force field. The 200 ns times in MD simulations were adopted to extract representational inputs to analyze the solvation layer and its interference where applicable In TD-DFT using BLYP and 6-311G(d). The molecular dynamics calculations were performed using the GROMACS 4.5 package.

Key-words: ZnNc, ZnPc, Molecular Dynamics, Aggregation
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