Title: **Designing new tunable materials for organic electronic devices**
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In this work we use computational chemistry to evaluate how an applied electric field can affect the conformation of a π-conjugated linker in 2D materials. To do this we use a model molecular system with different variations on its substituents and evaluate how an electric field can affect the energetic relative stability of their conformations through DFT calculations. Also, it will be explored in these model systems the validity of the first order approximation of the energy of a molecular system with an E-field applied.

These analyses on model systems are done in order to be representative at a small scale of the rotation of a linker in a dimer representation of a 2D-CORF (2D-CORFs are a relative new material). The knowledge acquired on the study of the model system will be used later to analyze the dimer of the 2D-CORF building block which it represents.

It has been found by the model system analysis that as higher is the dipole moment of the molecule is more susceptible to be changed its conformation. On other hand, the results reveal that the first order approximation works better as lower is the polarizability of the substituents, Fluorine is found to be the substituent with less error and because of this, it will be the substituent used in the following step of the study.

Finally, we designed a dimer of a 2D-CORF building block and carried out DFT calculations about the energy related to the rotation of the linker in the singlet and triplet states of the dimer. Moreover, it has been analyzed the strength of the magnetic interactions at all the possible conformations of the linker, related to the calculated energy gap of the multiplicity states. It has been found that the strength of the magnetic interactions changes at different conformations. In addition, has been used the first order approximation to predict the behavior of the dimer in an electric field and it has been targeted the conformation with highest magnetic interactions. Finally, it has been proved that magnetic properties in the material studied can be tuned by an applied electric field.

Keywords: computational chemistry, dimer, organic radical, DFT, model system, electric field, magnetism, first order approximation.