

## Supporting Information

### Modeling Charge Transport of Discotic Liquid-Crystalline Triindoles: The Role of Peripheral Substitution

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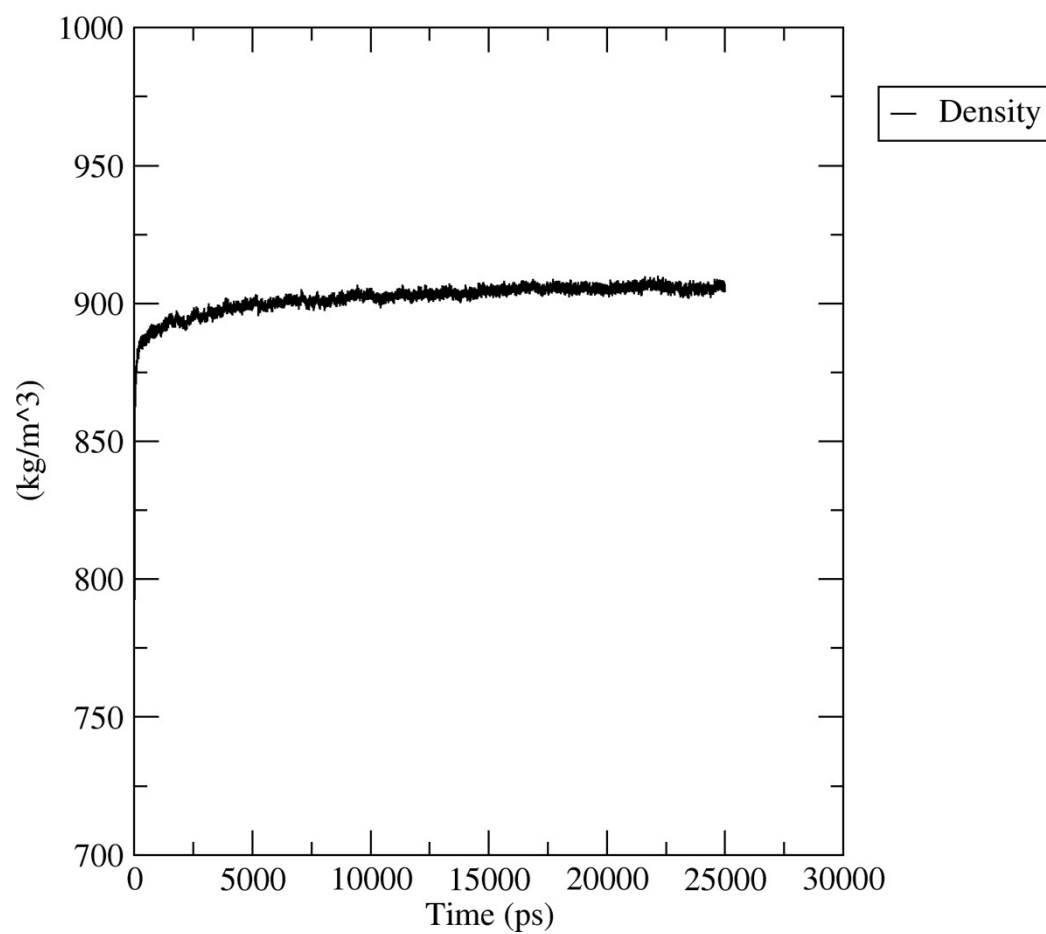
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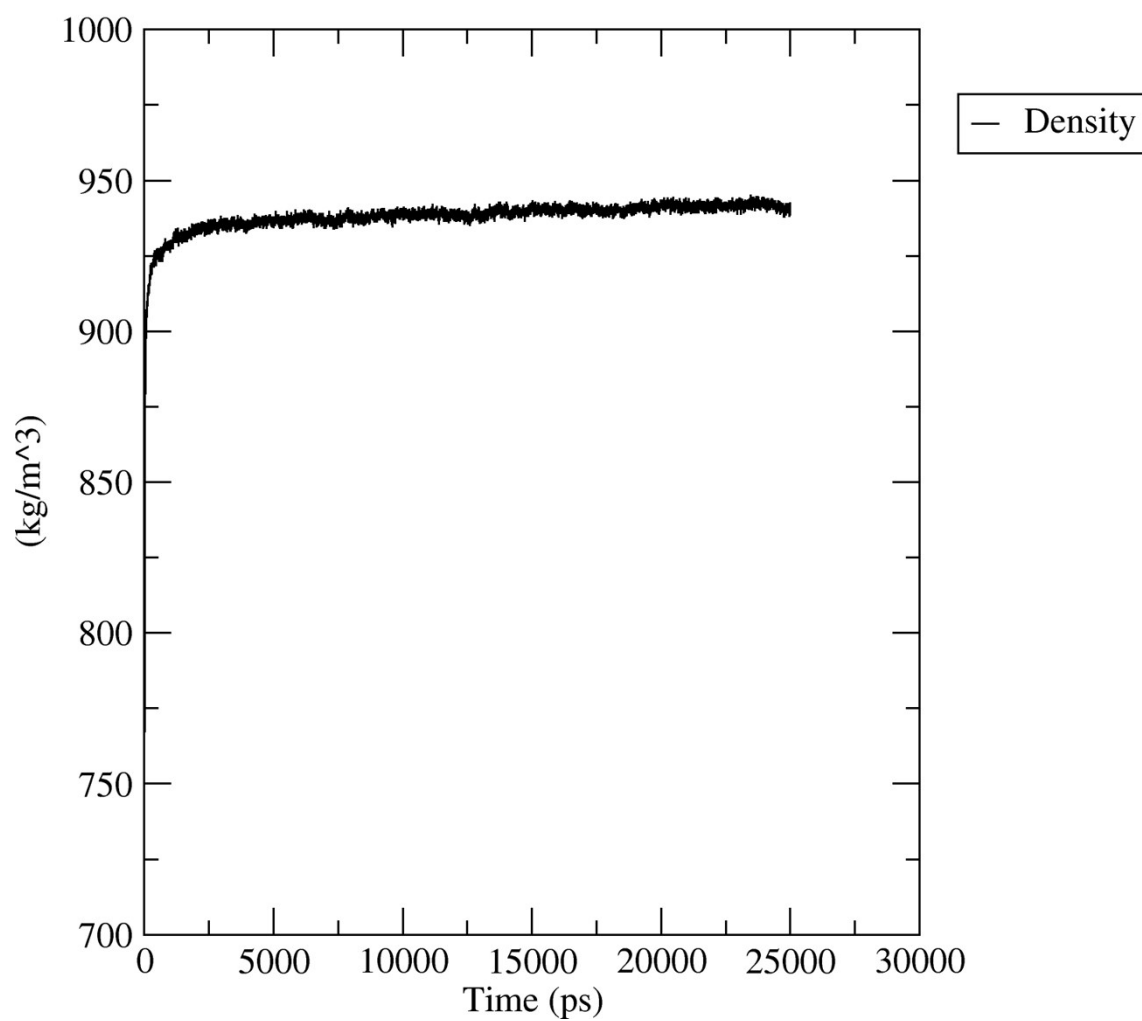
## MD SIMULATION

## Gromacs Energies



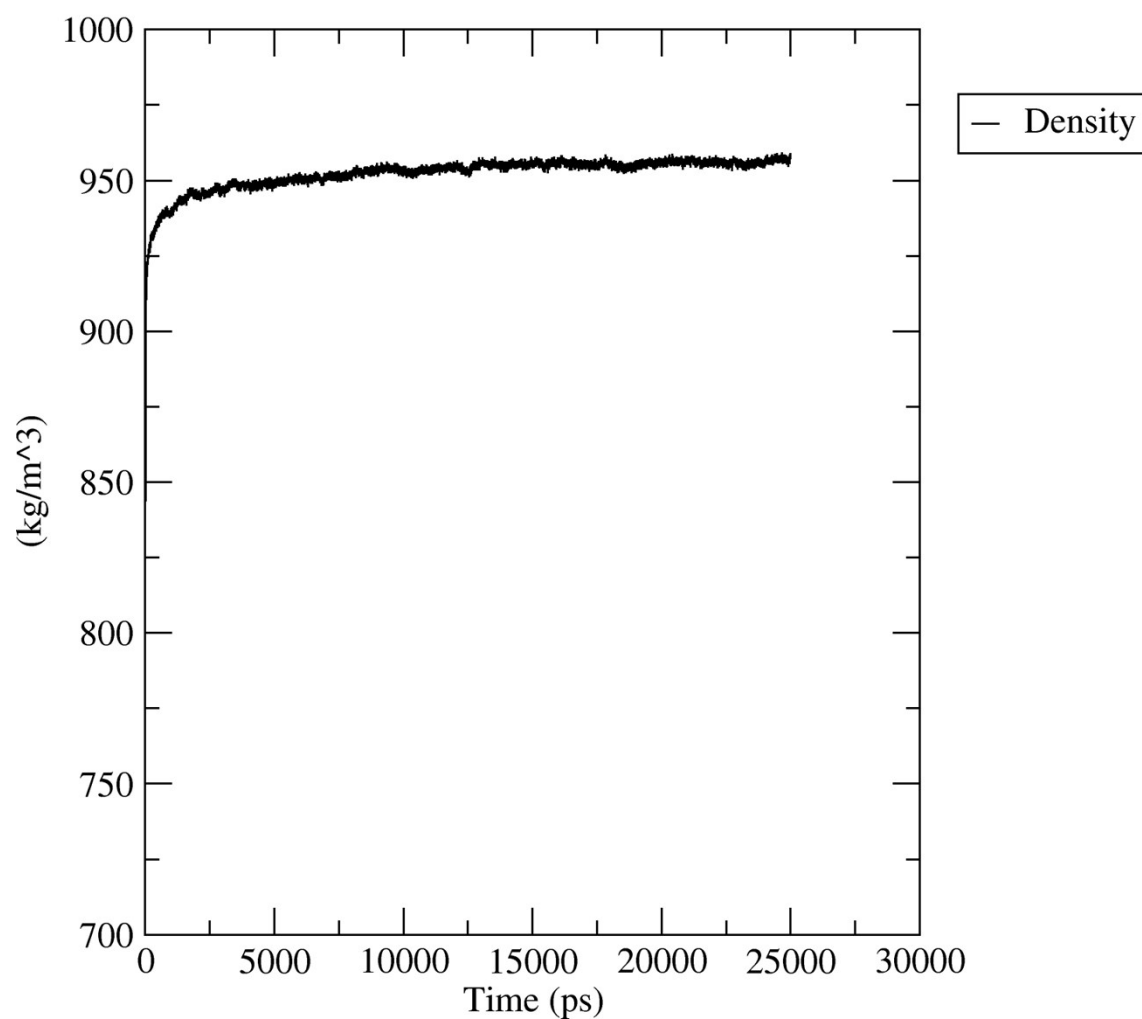
**Figure S1.** Density evolution for the NPT simulation (as described at page 4, section MM/MD) for model1.

## Gromacs Energies

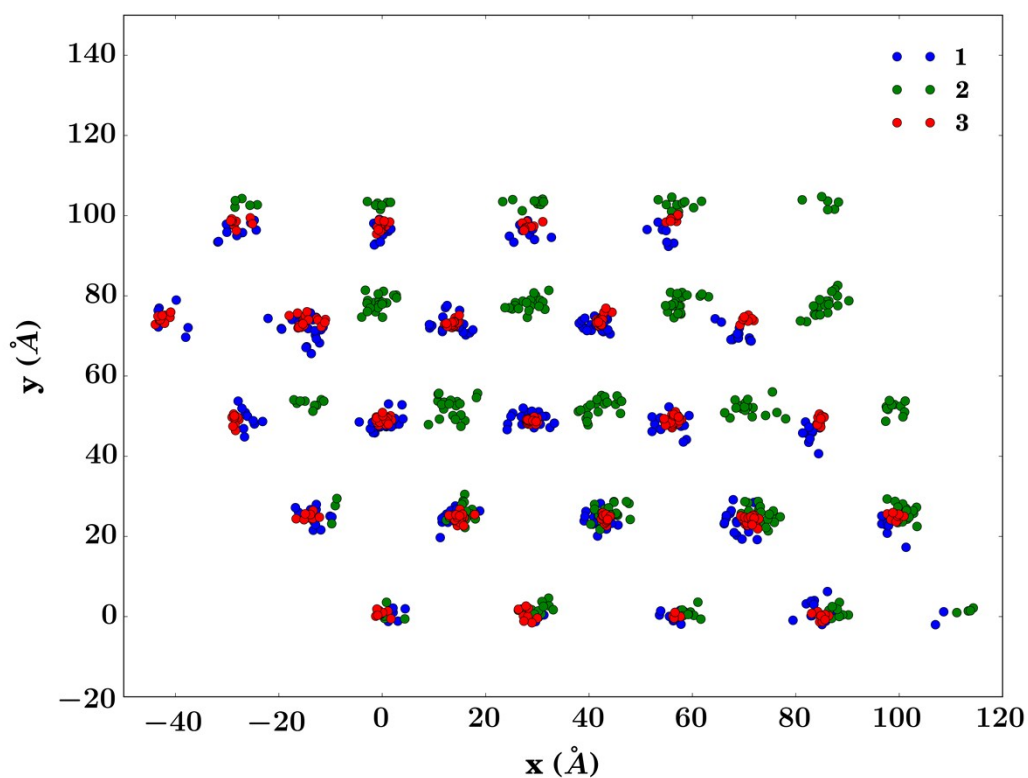


**Figure S2.** Density evolution for the NPT simulation (as described at page 4, section MM/MD) for model2.

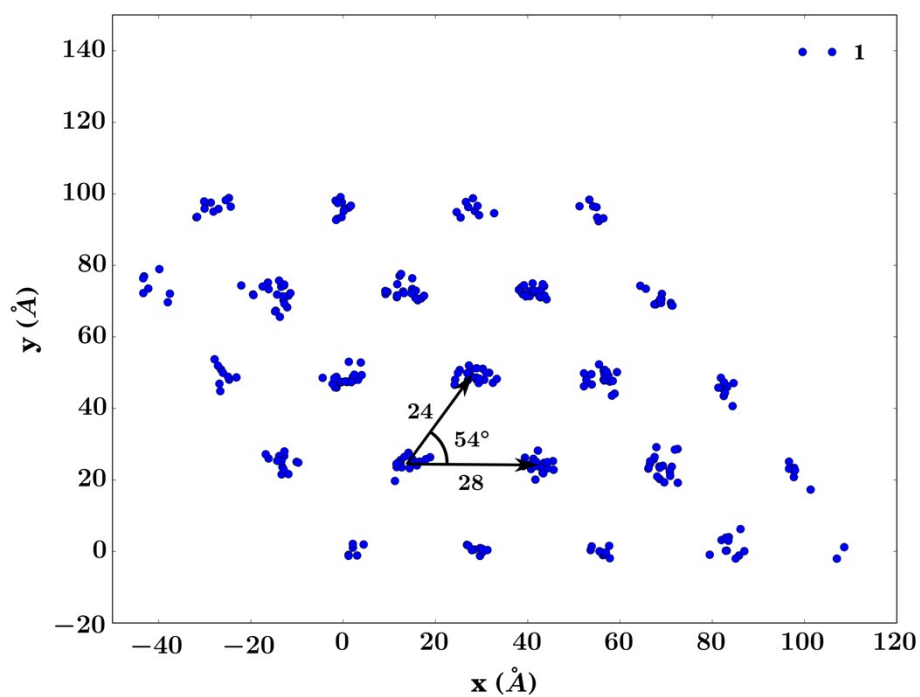
## Gromacs Energies



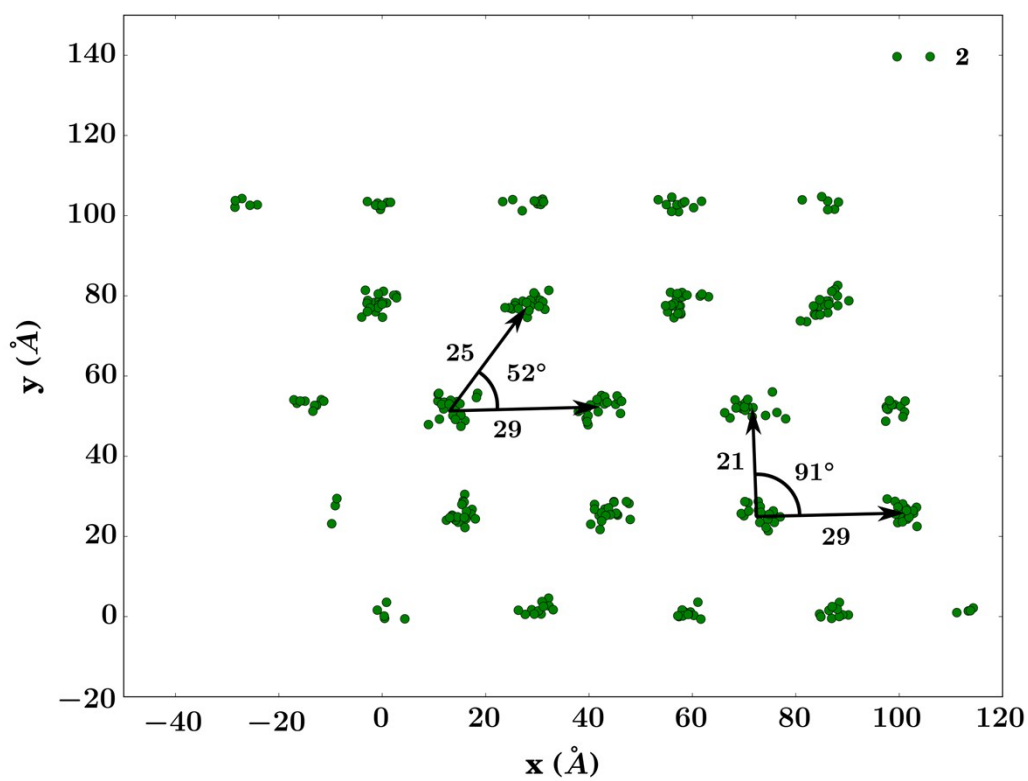
**Figure S3.** Density evolution for the NPT simulation (as described at page 4, section MM/MD) for model3.



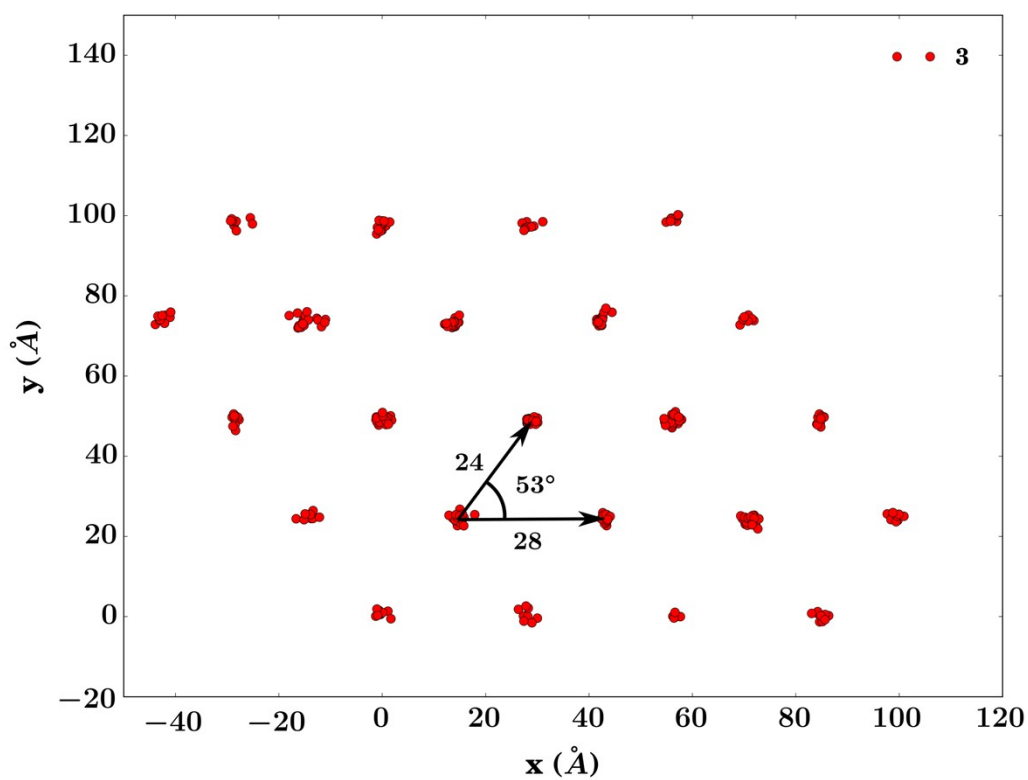
**Figure S4.** Visualization of the columnar structure of the 3 molecule species studied in the present paper, after MD equilibration. Projection on the xy plane of the core of the discotic molecules.



**Figure S5.** Visualization of the columnar structure for **1**.



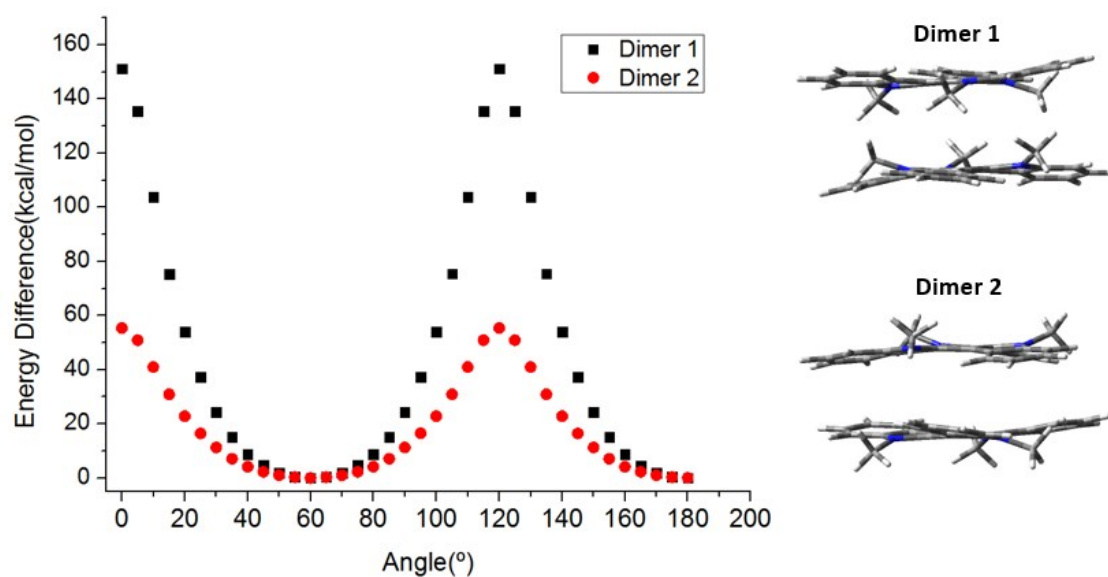
**Figure S6.** Visualization of the columnar structure of specie 2.



**Figure S7.** Visualization of the columnar structure of specie 3.

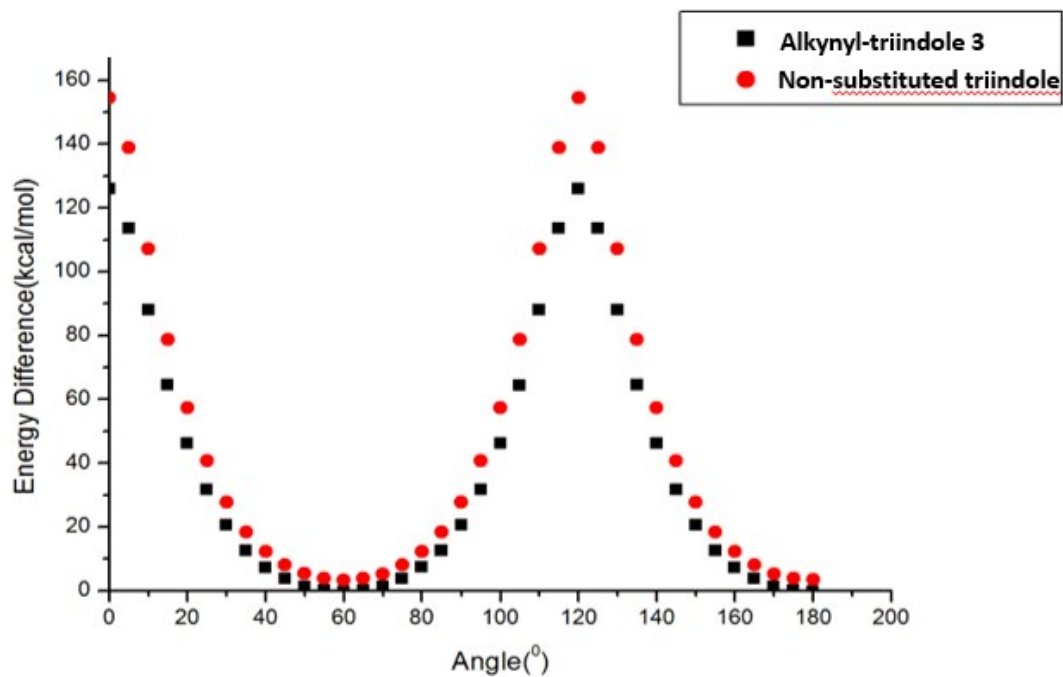
## DFT-calculated Potential Energy Surfaces

Here we report the calculated rigid potential energy surfaces (PES) in dimers formed by two *N*-methyl substituted triindole molecules as a function of rotation of one molecule around the stacking axis. Figure 8 shows the comparison between model dimers of a non-peripherally substituted *N*-methyl triindole adopting the two different conformations found in the crystal structure (named as cofacial dimer 1 and cofacial dimer 2 conformations). As noted, in both cases, the PES energy minimum is located at 60° with the maximum found for the cofacial configuration. It is also interesting to note that the energy barrier obtained between the cofacial and 60° staggered conformation is slightly affected by the peripheral substitution (see Figure 9 for the comparison between a dimer model of a non-peripherally substituted triindole and alkynyl-substituted triindole 3). Therefore, the PES calculations are in agreement with the electrostatic surface potential previously reported in the manuscript, giving support to the 60° rotated structure found in the supramolecular arrangement.



**Figure S8.** Rigid potential energy surface, computed at the  $\omega$ B97XD/6-31G\*\*, in dimers formed by two *N*-methyl substituted triindole molecules as a function of rotation of one molecule around the stacking axis. The intermolecular distance is set at 3.65 Å, the average intermolecular separation found in the *N*-methyl substituted triindole crystals along the  $\pi$ -stacks.





**Figure S9.** Rigid potential energy surface, computed at the  $\omega$ B97XD/6-31G\*\*, in dimers formed by two non-peripherally substituted triindole molecules and two alkynyl-substituted triindoles **3** as a function of rotation of one molecule around the stacking axis. The intermolecular distance is set at 3.65 Å.