Electronic Supplementary Information

A Theoretical study on lidocaine solubility in deep eutectic solvents

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The general form of the applied force field is:

\[ E = \sum_{bonds} k_b (r - r_{eq})^2 + \sum_{angles} k_\theta (\theta - \theta_{eq})^2 + E_{tor} \]

\[ + \sum_i \sum_j \left\{ 4\varepsilon_{ij} \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right\} + \frac{q_i q_j e^2}{4\pi\varepsilon_0 r_{ij}} \]

Graphene was maintained as rigid along the simulations, thus dihedrals \( E_{tor} \) were null for all the molecules.

Improper dihedrals were described according to:

\[ E_{improper} = k_{\phi}(\phi-\phi_0)^2 \]

### Table S1 Force field parameterization used for MD simulations

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S14
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