## Magnetic Field Induced Alignment of Macroradical Epoxy for Enhanced Electrical Properties

-Supplementary Information -

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Fig. S1: Illustration of the polarized IR microspectroscopy approach, where  $\Theta$  corresponds to the maximum absorbance angle.



Fig. S2: Quantum Computational Modelling Approach

| 1.<br>2.<br>3.       | Create rectangular prism-shaped unit cells (i.e., Back-<br>Front, Head-Front, and Head-Back).<br>Define spacing dimensions.<br>Define the unit cell's direction in line with the unit vector of<br>the transition dipole moment. | Preparation of the unit cells                   |                            |  |
|----------------------|--|---|----------------------------|--|
|                      |  | Development of<br>a lattice-based<br>model      | 1.<br>2.<br>3.<br>4.<br>5. | Create the lattice.<br>Define the required radical density.<br>Define the level of confidence bound (i.e., $\alpha$ =0.05).<br>Define the number of trials per radical density (i.e., 25 trials<br>each).<br>Set the non-nearest neighbor ATEO molecules' interaction<br>energies to zero during the simulation.                         |
| 1.<br>2.<br>3.       | Start polymerization at any location within the lattice-<br>based model.<br>Follow Standard Random Walk Algorithm in generating<br>random moves (i.e., sweeps).<br>Generate one move (i.e., sweep) at a time.                    | Generation of<br>the random<br>polymeric chain  |                            |  |
|                      |  | Checking of the<br>generated<br>polymeric chain | 1.<br>2.<br>3.             | <ul> <li>Ensure that each move acceptance is based on the standard random walk algorithm.</li> <li>Ensure that the polymeric chain's density should not fall beneath ~0.6 per nm<sup>-3</sup>.</li> <li>Ensure that the consecutive moves could not result in voids in the lattice-based model using the standard random walk</li> </ul> |
| 1.<br>2.<br>3.<br>4. | Calculate the average Percolation Span.<br>Calculate the average Radical Density.<br>Calculate Standard Deviation for each trial.<br>Calculate the level of confidence bound.  | Generation of<br>the required<br>calculations   | 4.                         | Ensure that random translation from an occupied lattice<br>site (i.e., a unit cell) to a neighboring one is attempted<br>while constrained by the direction of the transition dipole<br>moment vector.   |

Fig. S3: Monte Carlo Simulation Approach



 Table S1: Summary of all possible combinations along with binding energy curves and minimum energy.





|      |               |              |  | Minimum                   |
|------|---------------|--------------|--|---------------------------|
| S/N  | Configuration | Illustration | Binding Energy Curve   | Energy                    |
|      |               |              |  | (kcal mol <sup>-1</sup> ) |
| 9.0  | Head-Back     |              | Public Provide state sta | -121.91                   |
| 10.0 | Head-Edge1    |              | Unstable   | N/A                       |
| 11.0 | Heade-Edge2   |              | Unstable   | N/A                       |
| 12.0 | Head-Head     |              | Unstable   | N/A                       |