Electronic Supplementary Material (ESI) for Soft Matter.

Magnetic Field Induced Alignment of Macroradical Epoxy for Enhanced Electrical Properties

-Supplementary Information -

Ahmed Al-Qatatsheh,[a] Jaworski C. Capricho,[a] Jitraporn (Pimm) Vongsvivut,[b] Mark J. Tobin,[b] Saulius Juodkazis,[c] Nishar Hameed*[a]

[a] School of Engineering, Swinburne University of Technology, Melbourne VIC 3122, Australia.

[b] Infrared Microspectroscopy (IRM) Beamline, ANSTO – Australian Synchrotron, 800 Blackburn Road, Clayton, Victoria 3168, Australia.

[c] Optical Sciences Centre and ARC Training Centre in Surface Engineering for Advanced Materials (SEAM), Faculty of Science, Engineering and Technology, Swinburne University of Technology, Hawthorn, VIC 3122, Australia

[*] E-mail: nisharhameed@swin.edu.au, aalqatatsheh@swin.edu.au

Content

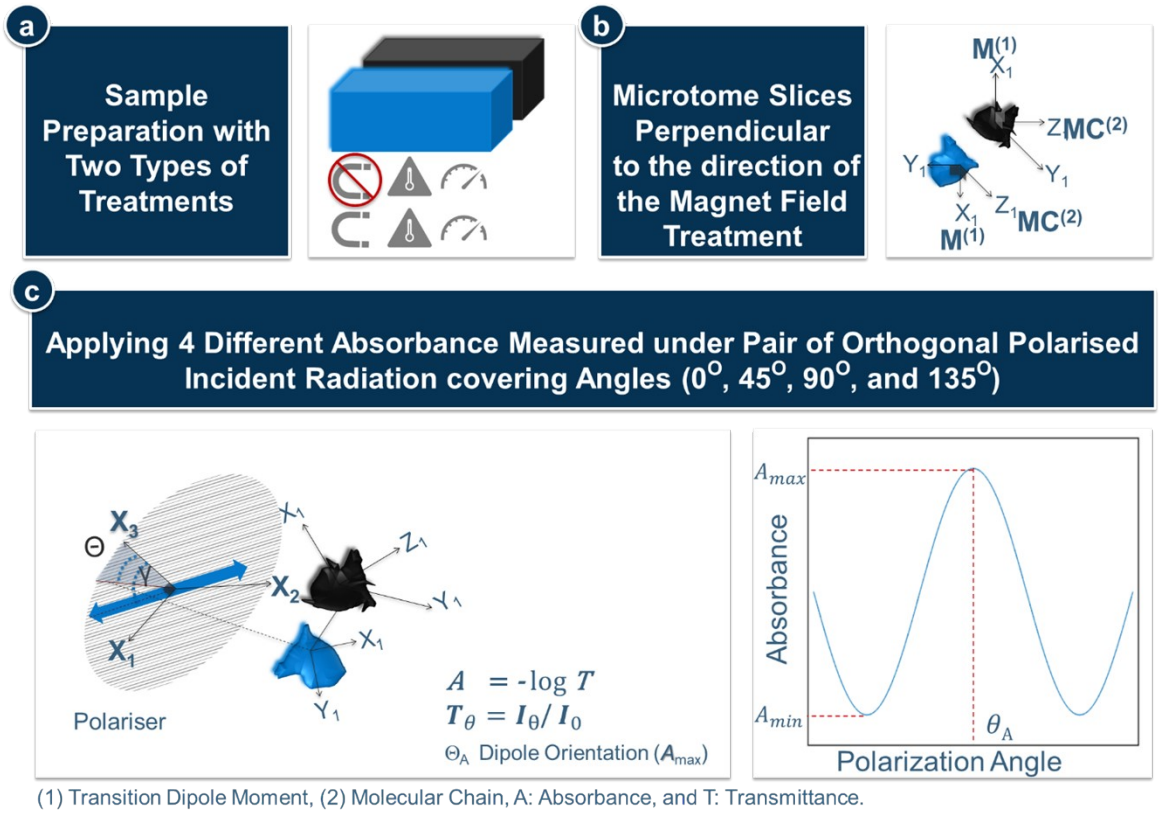


Fig. S1: Illustration of the polarized IR microspectroscopy approach, where Θ corresponds to the maximum absorbance angle.

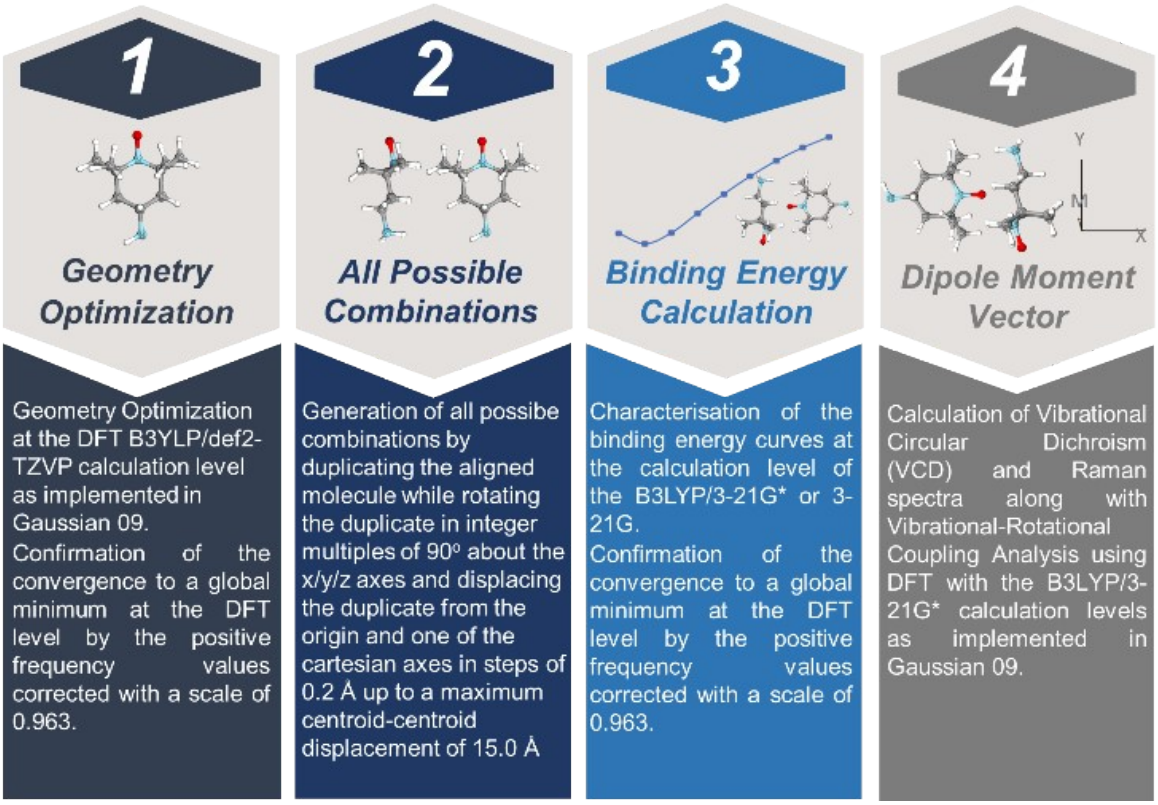


Fig. S2: Quantum Computational Modelling Approach

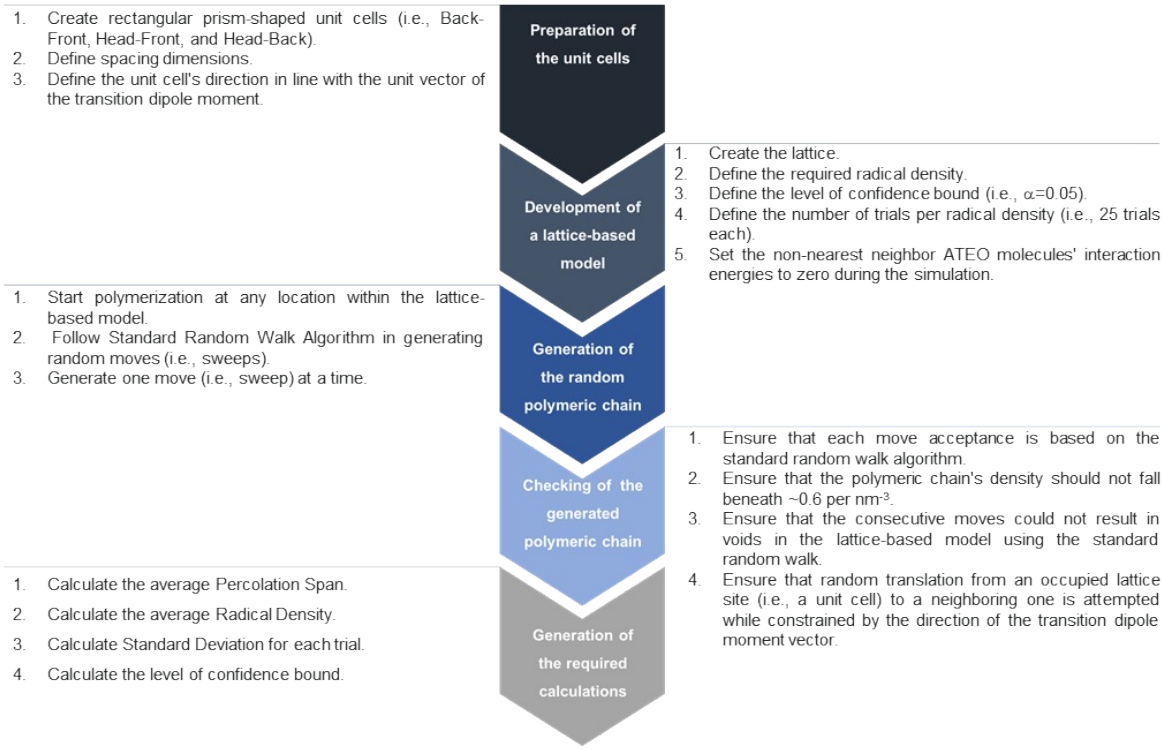
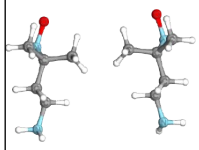
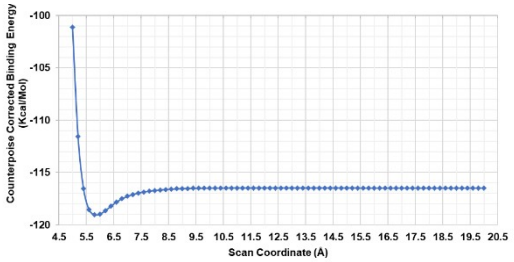
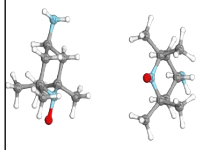
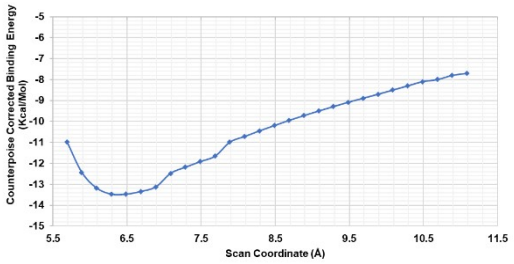
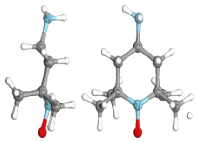
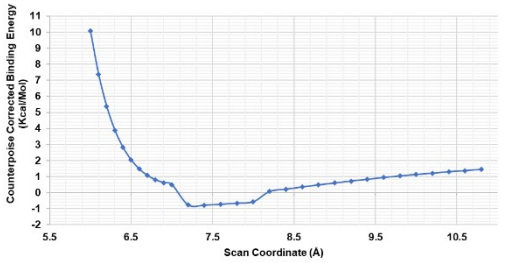
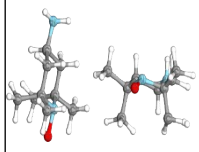
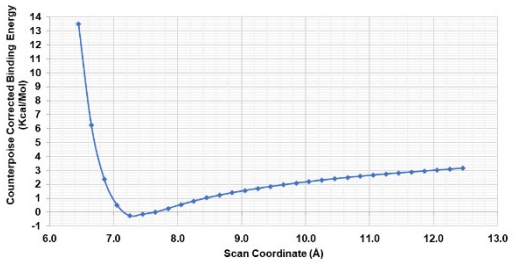
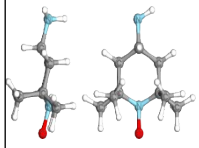
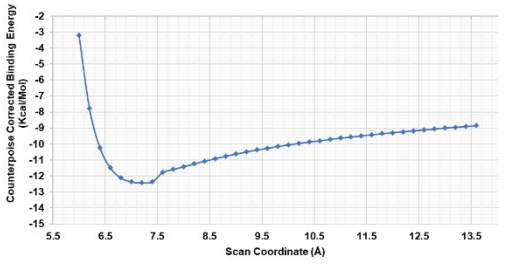
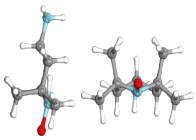
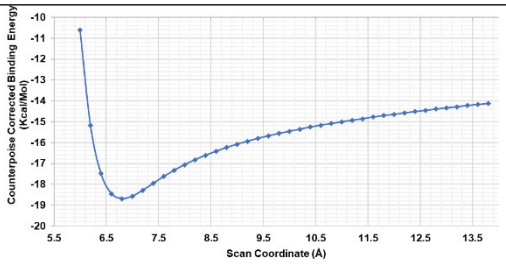
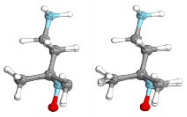
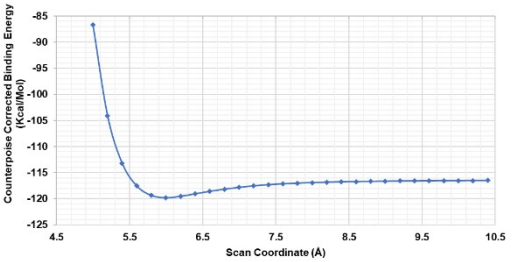
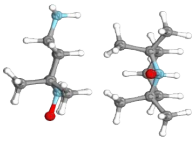
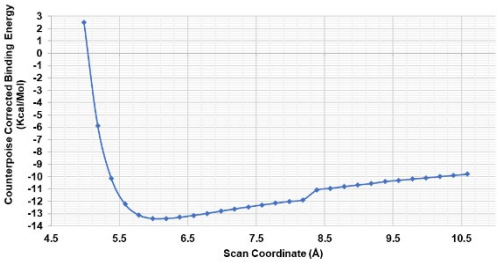
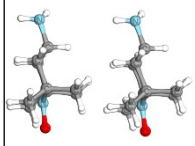
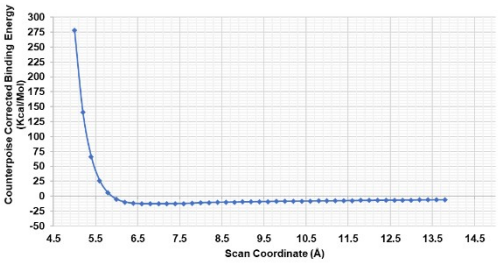
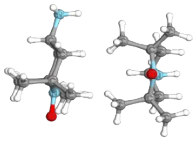
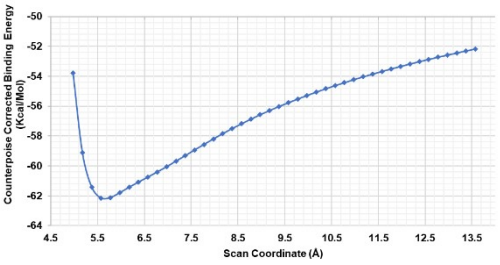
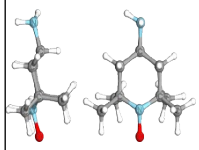
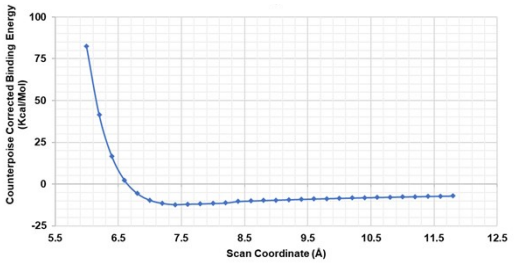
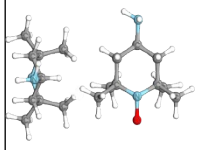
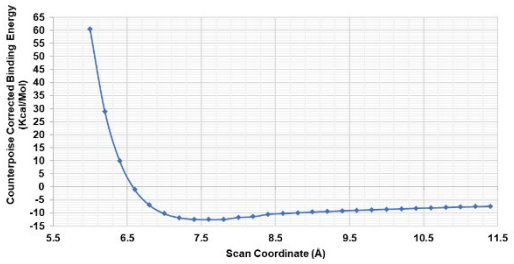
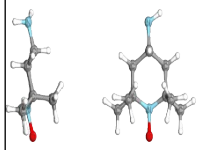
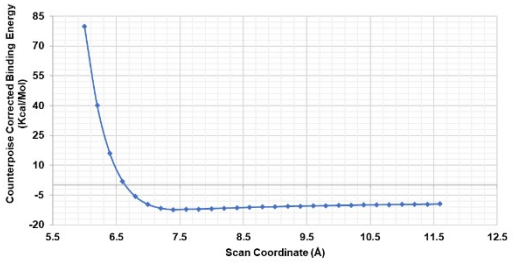
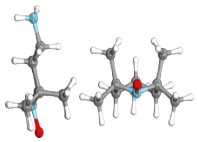
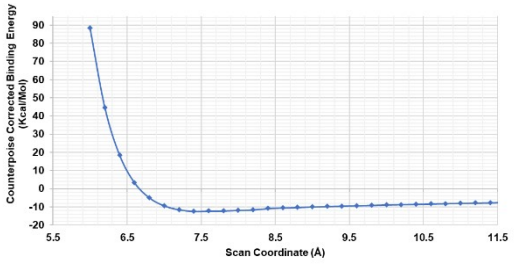
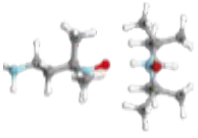
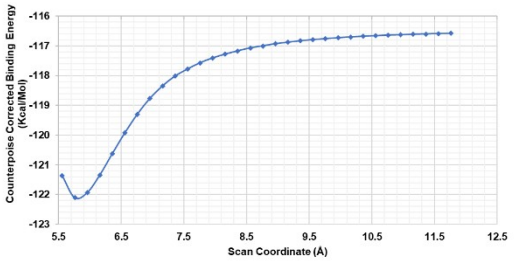


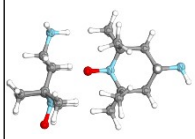
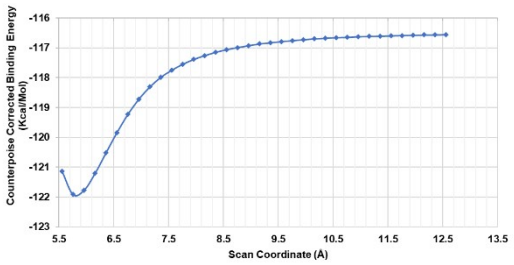
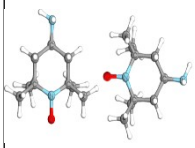
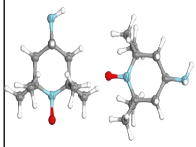
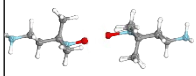
Fig. S3: Monte Carlo Simulation Approach

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

S/N	Configuration	Illustration	Binding Energy Curve	Minimum Energy (kcal mol^{-1})
1.0	Back-Back			-119.04
1.1	Back-Back(90)			-13.48
2.0	Back-Edge1			-0.78
2.1	Back-Edge1(90)			-0.27
3.0	Back-Edge2			-12.41
3.1	Back-Edge2(90)			-18.69

S/N	Configuration	Illustration	Binding Energy Curve	Minimum Energy (kcal mol^{-1})
				
4.0	Back-Front			-119.80
4.1	Back-Front(90)			-13.40
5.0	Front-Front			-12.98
5.1	Front-Front(90)			-62.16

S/N	Configuration	Illustration	Binding Energy Curve	Minimum Energy (kcal mol^{-1})
6.0	Front-Edge1			-12.23
6.1	Front-Edge1(90)			-12.55
7.0	Front-Edge2			-12.37
7.1	Front-Edge2(90)			-12.34
8.0	Head-Front			-122.11

S/N	Configuration	Illustration	Binding Energy Curve	Minimum Energy (kcal mol^{-1})
9.0	Head-Back			-121.91
10.0	Head-Edge1		Unstable	N/A
11.0	Heade-Edge2		Unstable	N/A
12.0	Head-Head		Unstable	N/A