Supplementary Material (ESI) for CrystEngComm

Predicting crystalline polyamic acids as precursors to porous polyimides

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Supplementary information

The networks described were constructed using the Materials studio visualiser. The systems were fully minimised using the Discover minimisation package using the COMPASSS forcefield with no symmetry group constraints imposed. van der Waals interactions were treated using atom based summation whilst coulombic interactions were treated using Ewald summation a cutoff distance of 9.50 Å was used for all models. Models **A1** and **A3** were further geometry optimised using the DMol^3 density functional theory module using the GGA functional and BLYP basis set with a medium setting.

	meta	para
A1	-1176.37	-1176.39
A3	-3296.92	-3296.88
A5	-1087.96	-1095.45

Table 1. The absolute energies of the six potential polyamic acid framework intermediates for polyimides with distinct network topologies. A1 and A2 show the absolute energies calculated using the DMol^3 density functional theory module using the GGA functional and BLYP basis set with a medium setting. A5 absolute energy was calculated using the Discover minimisation package using the COMPASSS forcefield.