Computer simulation study of the materials properties of intercalated and exfoliated poly(ethylene)glycol clay nanocomposites

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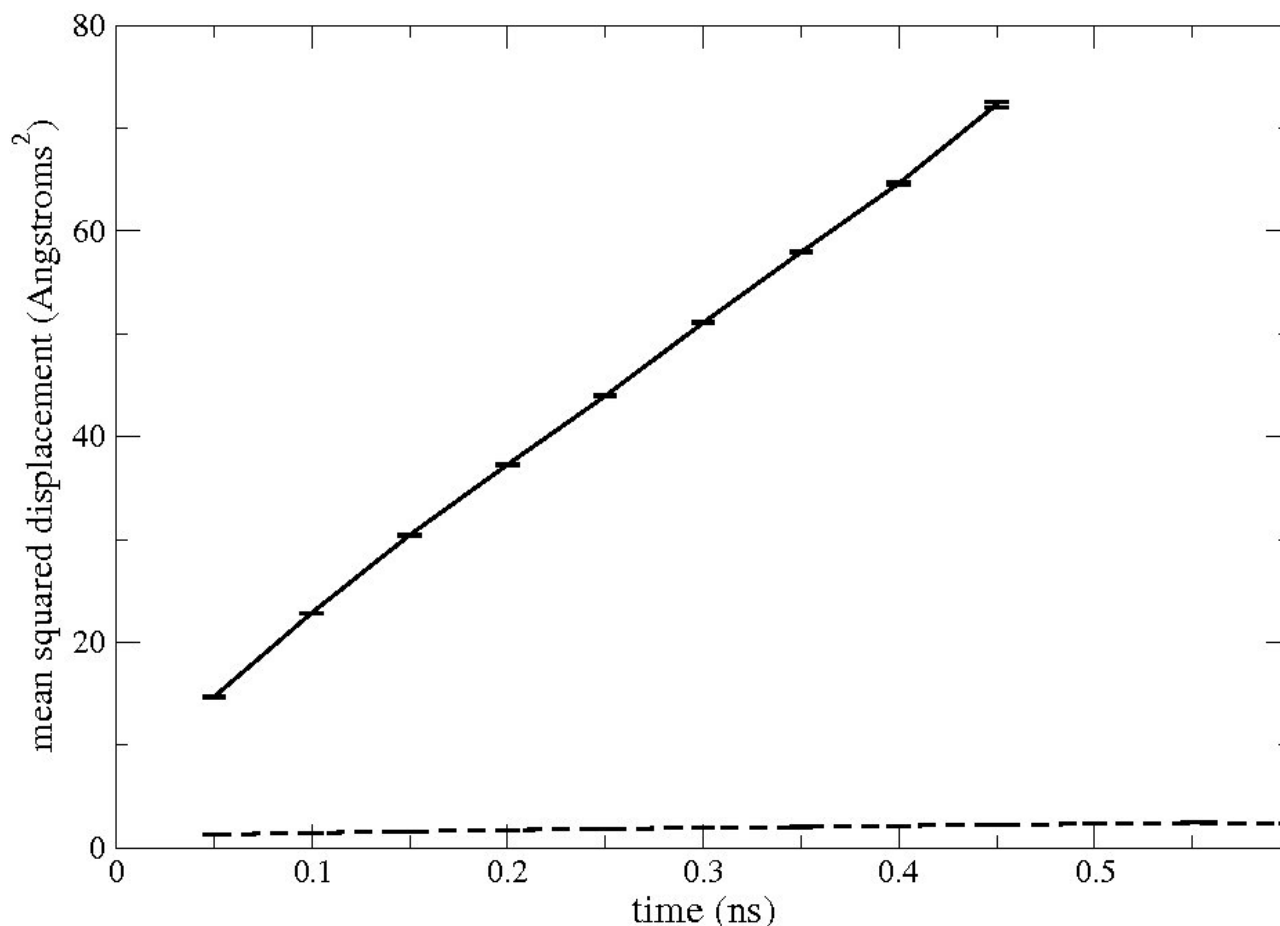20 Gordon Street, London, WC1H 0AJ, United Kingdom.

Figure S1: The mean squared displacement of PEO backbone atoms during pre-equilibration annealing molecular dynamics simulations at 500K of system I (solid line). Also shown is the mean-squared displacement at 300K (dashed line). We see much more motion at the higher temperature, allowing the system to explore configurational space.
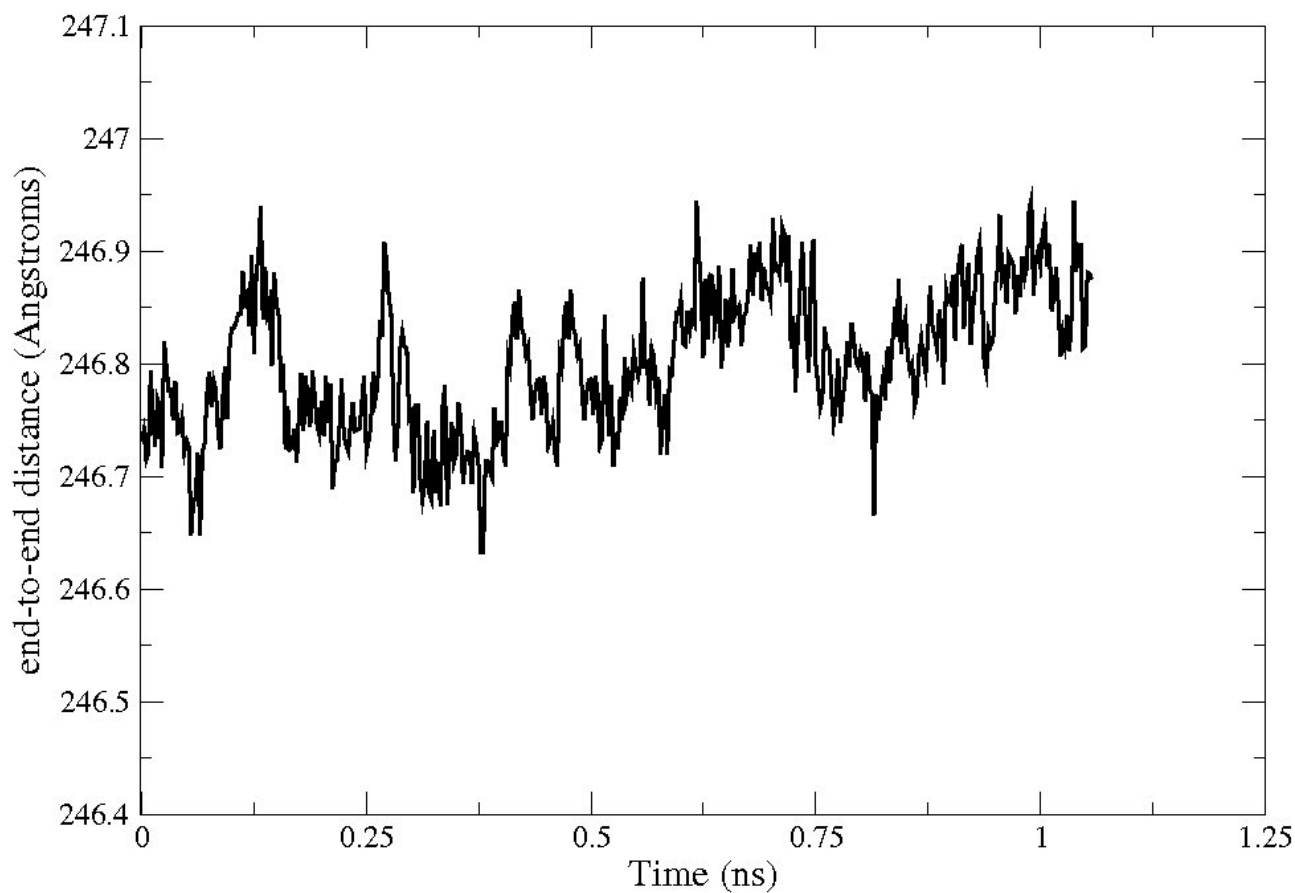
Figure S2: The end-to-end distance of PEO chains as a function of time over the last 1.0ns of simulation at 300K of the exfoliated clay system {\bf (I)}. We see there is very little drift in the value.
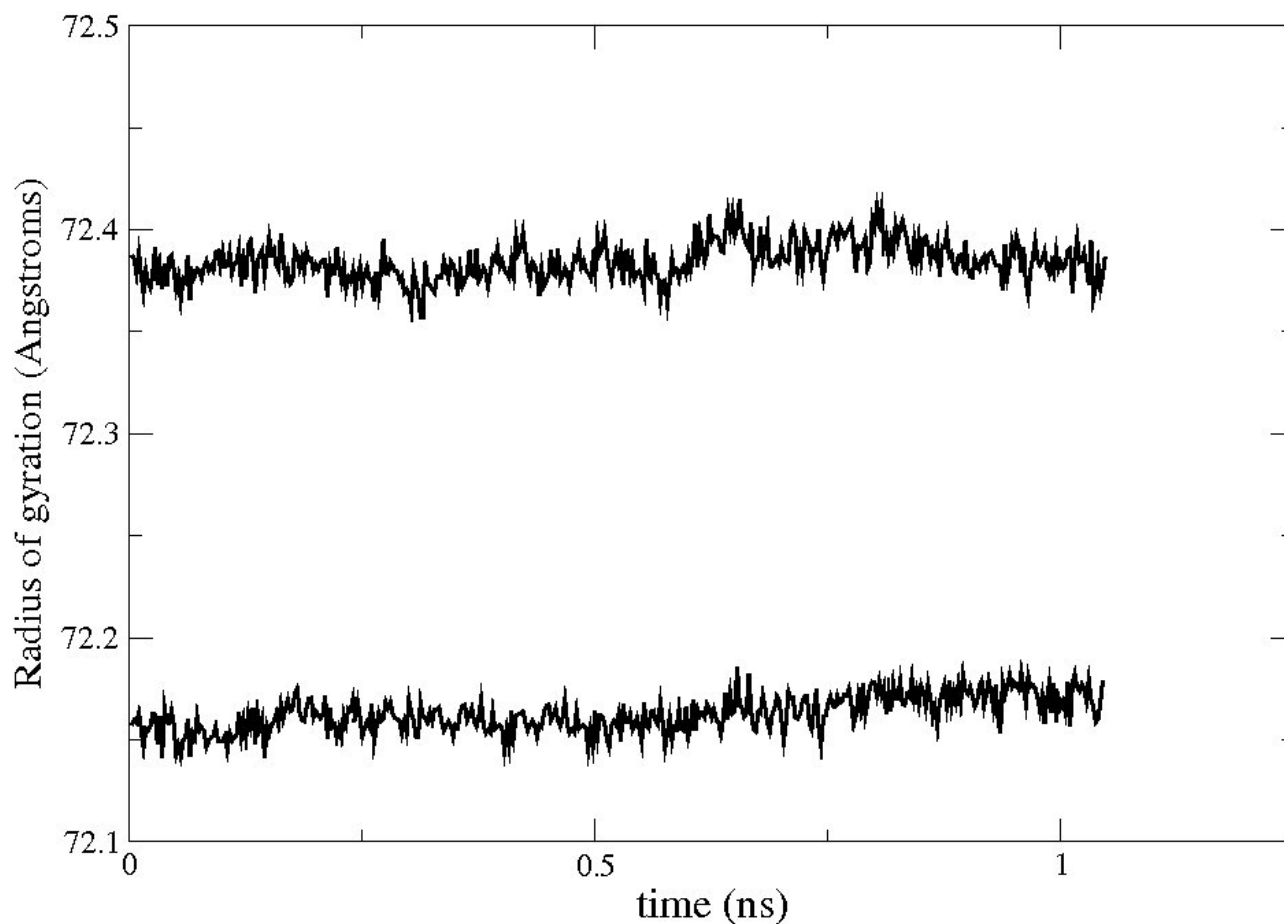
Figure S3: The radius of gyration of PEO chains in the layer closest to the clay surface (upper curve) and the layer furthest from the clay sheet (lower curve) as a function of time over the last 1.0ns of simulation at 300K of the exfoliated clay system I. We see there is negligible drift in these