Supplementary Information for Computer Simulation Study of the Structural Stability and Materials Properties of DNA-Intercalated Layered Double Hydroxides

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Also included are MPEG animations of height functions of Systems (I-III). Height functions are found for one LDH layer intercalated with DNA from snapshots taken during 1.5ns of MD simulation at 2ps intervals. AtomEye visualizations of the MD trajectories for 0-1.5ns of Systems (I-III) are also provided. All height functions and visualizations represent simulations carried out at 300K and 1 atm.

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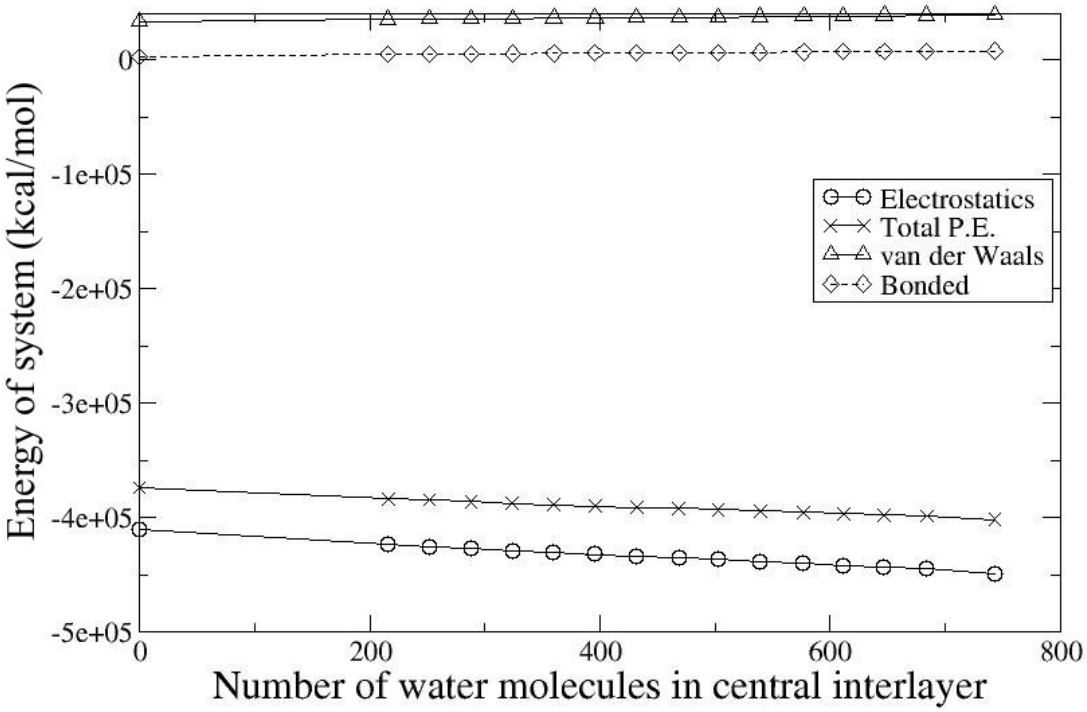


Figure 1: Breakdown of potential energy into it components for System I at different hydration states at 300K, averaged over 1ns of MD simulation. The electrostatic interaction is the dominant one between the DNA and LDH. Water content is varied in the interlayer containing DNA as a function of $[Mg_2Al(OH)_6]\cdot nH_2O$.

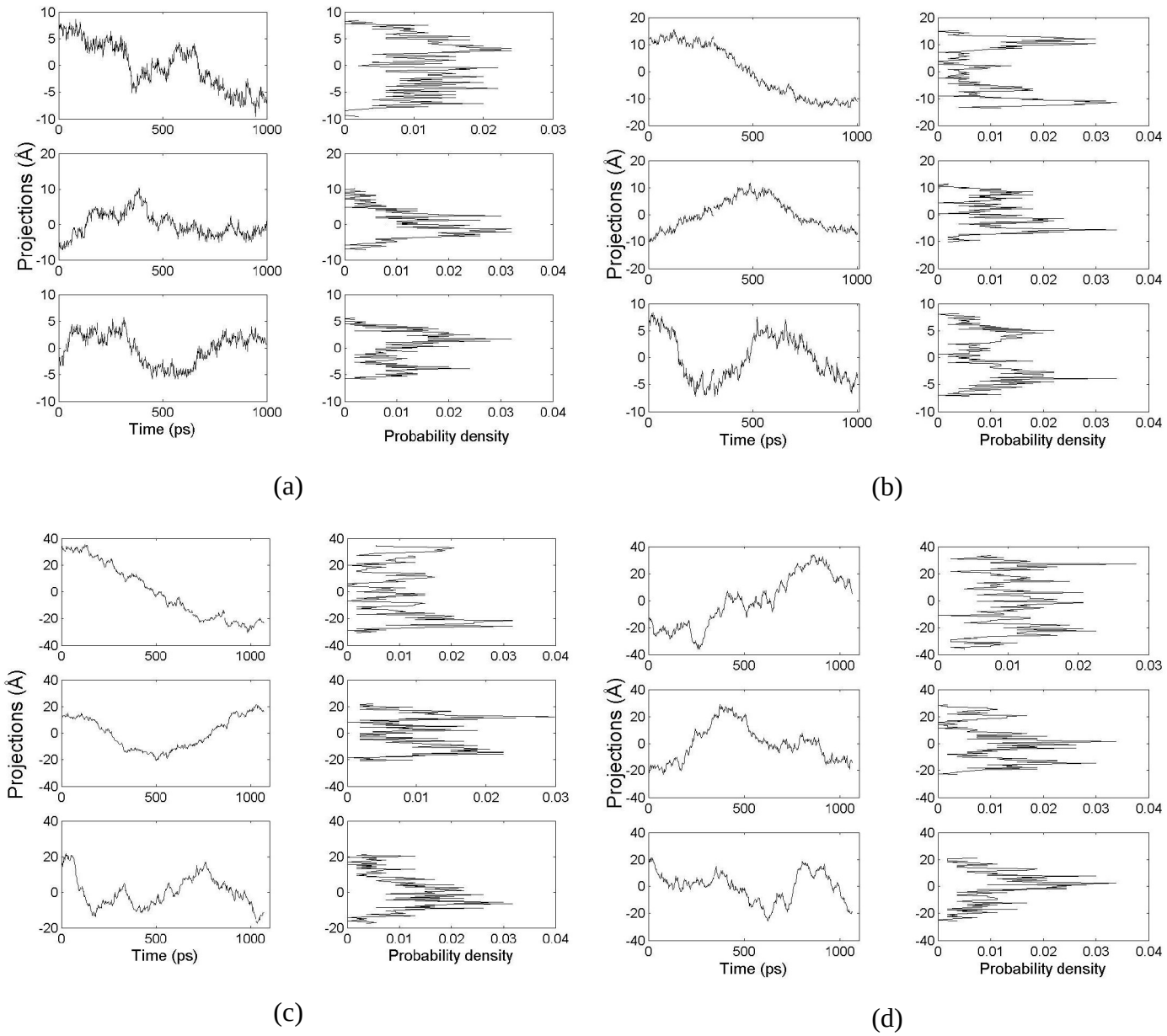
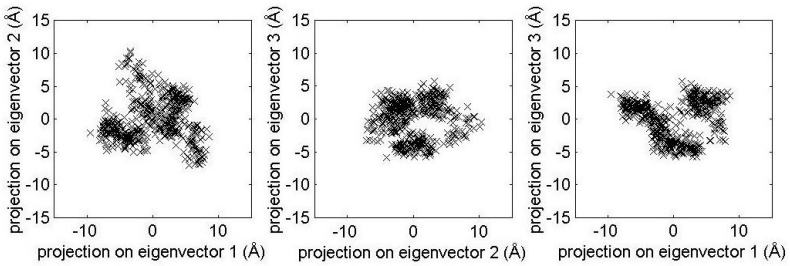
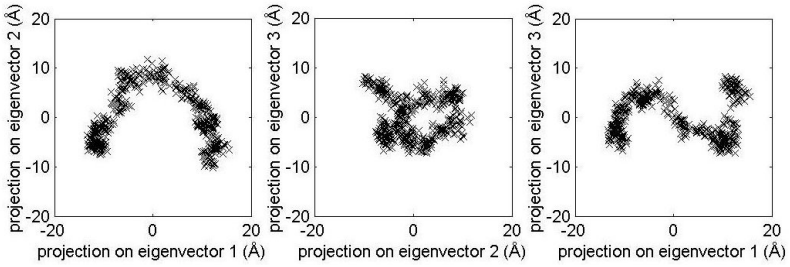


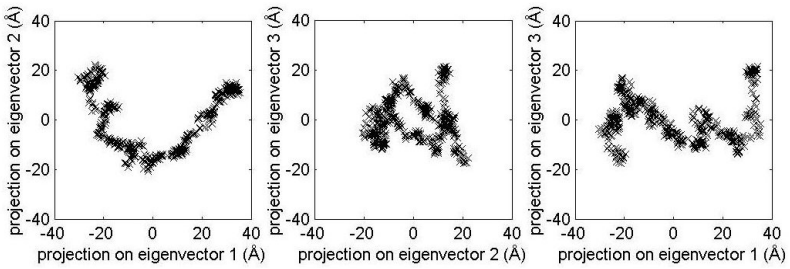
Figure 2: Motions along first three eigenvectors obtained from coordinates of the phosphate backbone of (a) System **I**; (b) System **II**; (c) System **III**; and (d) System **IV**. A bimodal probability distribution is observed for intercalated DNA; as the motion of intercalated DNA is extremely restricted the principal modes are heavily influenced by the thermal motion of the LDH sheets.



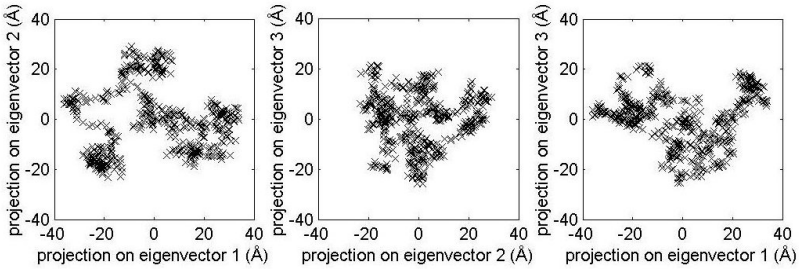
(a)



(b)

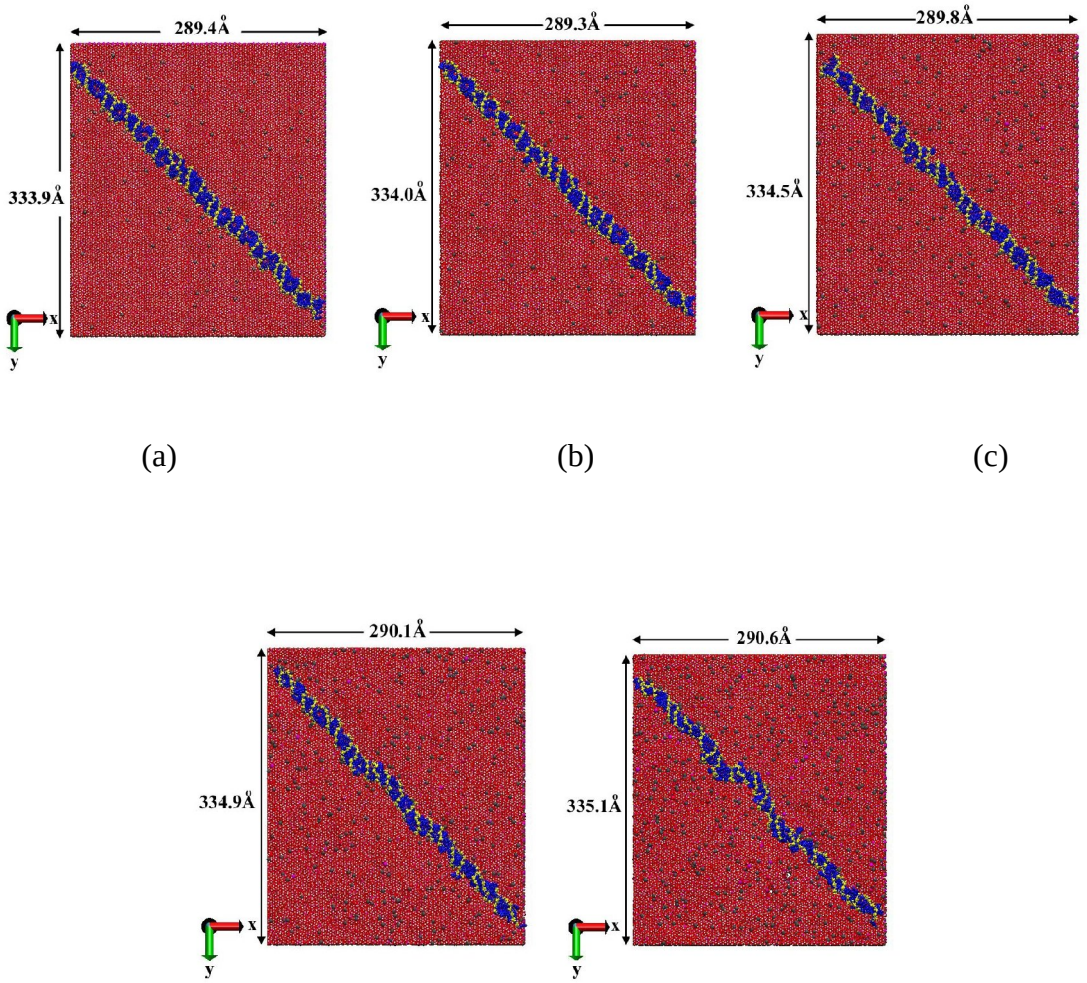


(c)



(d)

Figure 3: Projections of the trajectory from the phosphate backbone on planes defined by pairs of eigenvectors for (a) System **I**; (b) System **II**; (c) System **III**; and (d) System **IV**. Systems II and III show strong dependencies between the first three eigenvectors, suggesting that forces acting along these eigenvectors are coupled.



(a) (b) (c)

(d) (e)

Figure 4: AtomEye visualisations of final snapshot for System II at (a) 300K and 1 atm; (b) 350K and 1 atm; (c) 400K and 50 atm; (d) 450K and 100 atm; and (e) 500K and 100 atm. Water molecules and chloride ions have been not been displayed. Magnesium, aluminium, oxygen and hydrogen in the LDH sheets are represented as gray, pink, red and white spheres, respectively. The DNA strand has been coloured yellow to represent the phosphate backbone and blue for the sugar groups and base pairs. The DNA duplex is less restricted at higher temperatures, allowing the strand to supercoil.

Forcefield	Species	Charge (e)
ClayFF	Water hydrogen	0.4100
	Hydroxyl hydrogen	0.4250
	Water oxygen	-0.8200
	Hydroxyl oxygen	-0.9742
	Aqueous chloride ion	-1.0
	Octahedral aluminium	1.5750
	Octahedral magnesium	1.3600
Amber ff99	Phosphorus in phosphate groups	1.1659
	Oxygen in phosphate groups	-0.7761

Table 1: Atom type charges for LDH and phosphate groups in DNA atoms. The LDH charges are taken from the ClayFF forcefield, while the DNA charges are taken from the Amber ff99 forcefield.