

Supplementary information

## Wrapping/Unwrapping Transition of Double-Stranded DNA in DNA-Nanosphere Complexes Induced by Multivalent Anions

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Table 1: Various anion and cation concentrations used in our simulations. Here  $C_s$  and  $C_s'$  represent anion and cation concentrations, respectively

	$M^{1-}$				$M^{2-}$				$M^{3-}$				$M^{4-}$			
$C_s$ /mM	30.5	61.0	91.5	443.9	30.5	61.0	91.5	216.9	30.5	61.0	91.5	144.7	30.5	61.0	91.5	108.5
$C_s'$ /mM ( $M^{1+}$ )	61.0	91.5	121.9	464.6	91.5	152.3	213.3	464.6	121.9	213.3	304.7	464.6	152.3	274.2	396.1	464.6