Electronic supplementary information for

Notable Effect of Water in Excess Electron Attachment to Aqueous DNA Deoxyribonucleosides

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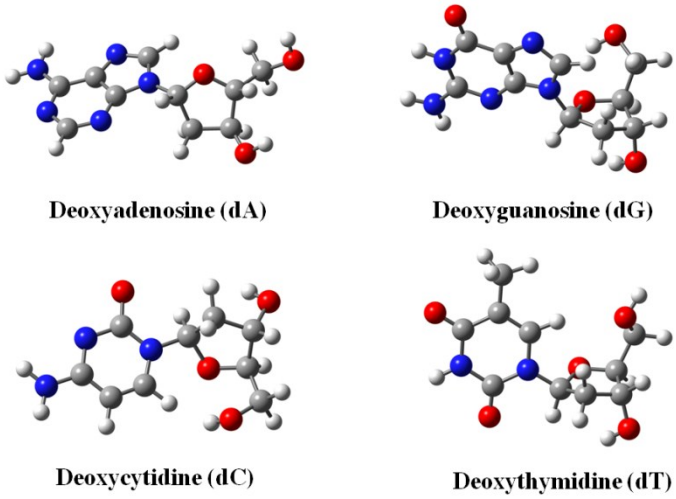
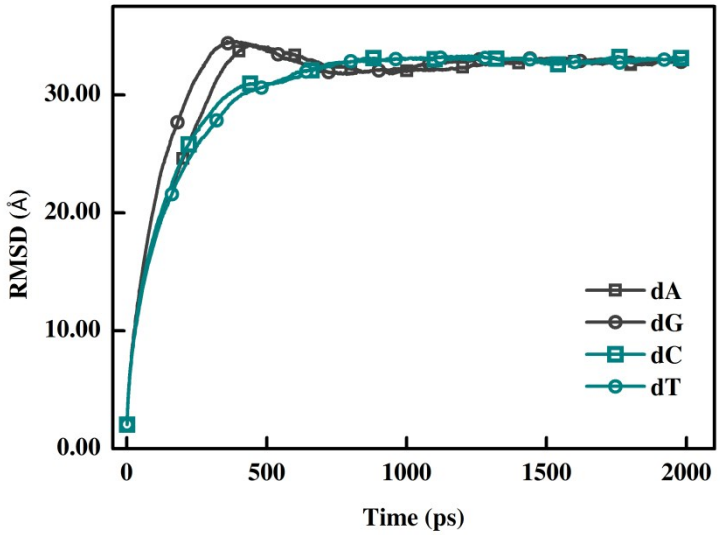


Figure S2. Root-mean-square Deviation (RMSD) of 2000 ps MD Simulations.



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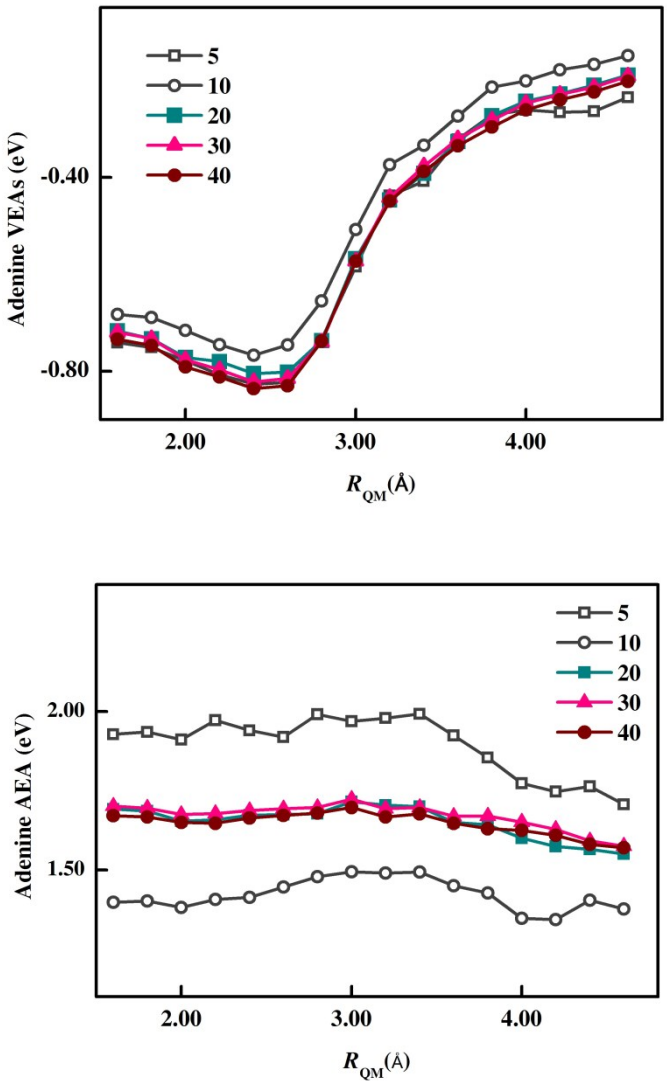


Figure S4. Vertical Electron Affinities (VEAs) of QM/MM Computations for 20 Snapshots.

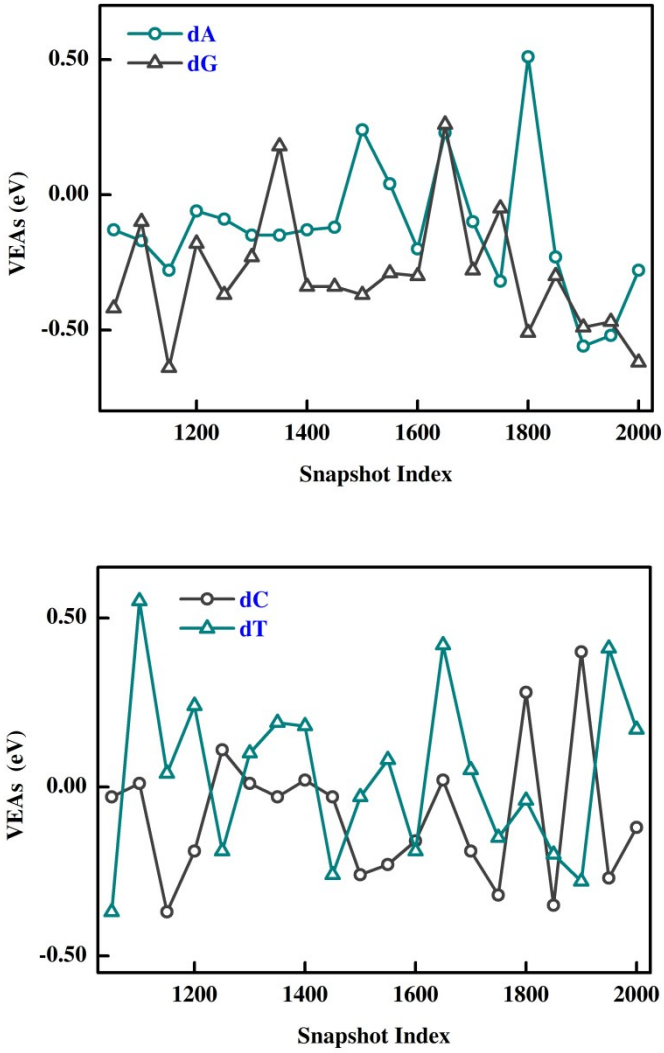
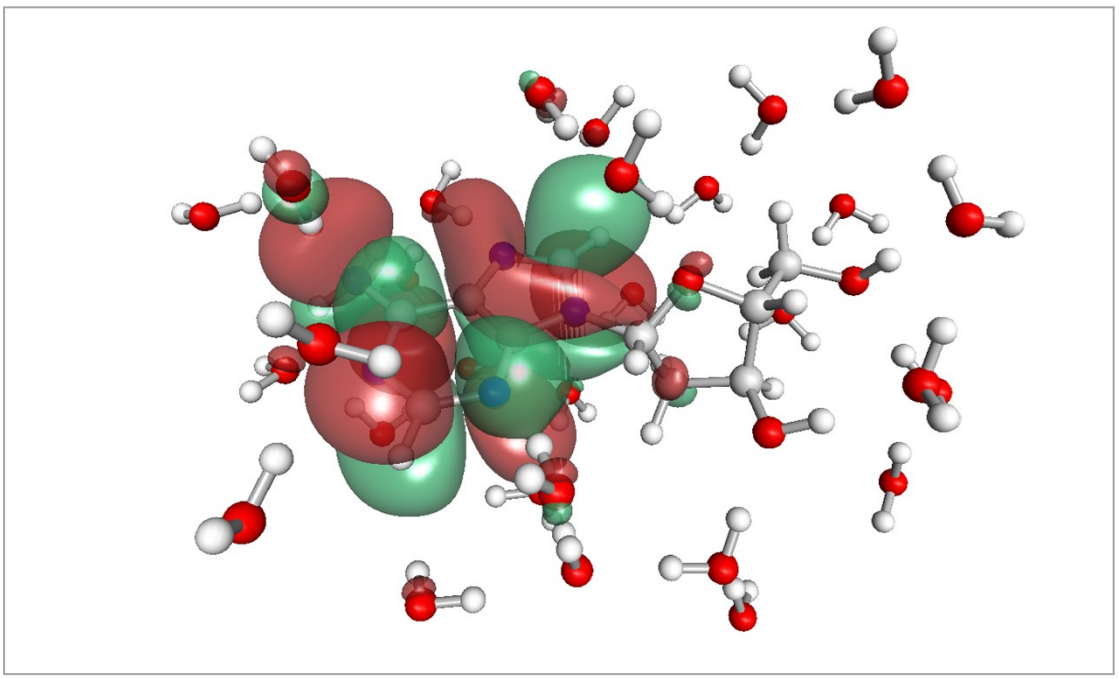


Figure S5. dA S1650 LUMO of Neutral Calculations.



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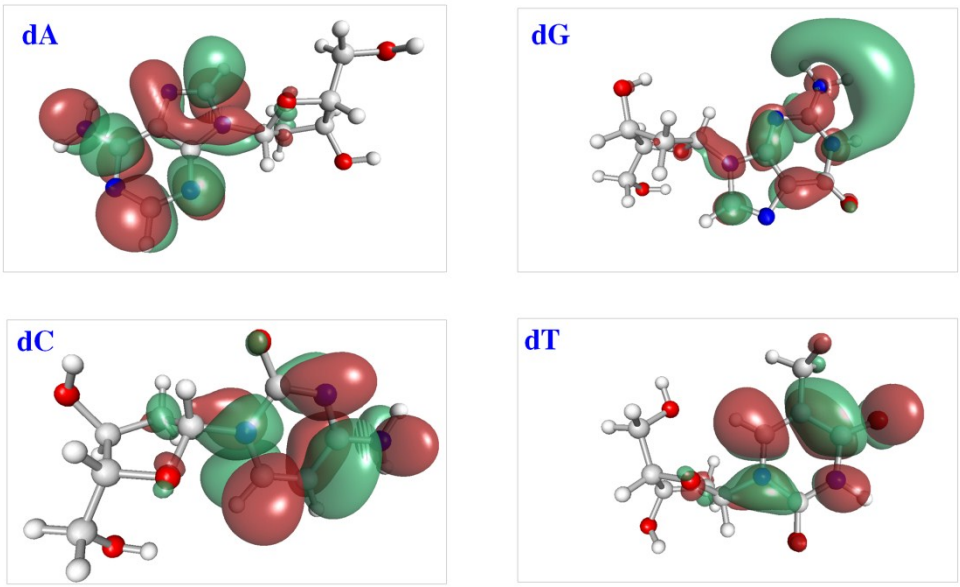

Figure S7. Adiabatic Electron Affinities (AEAs) of QM/MM Computations for 20 Snapshots.

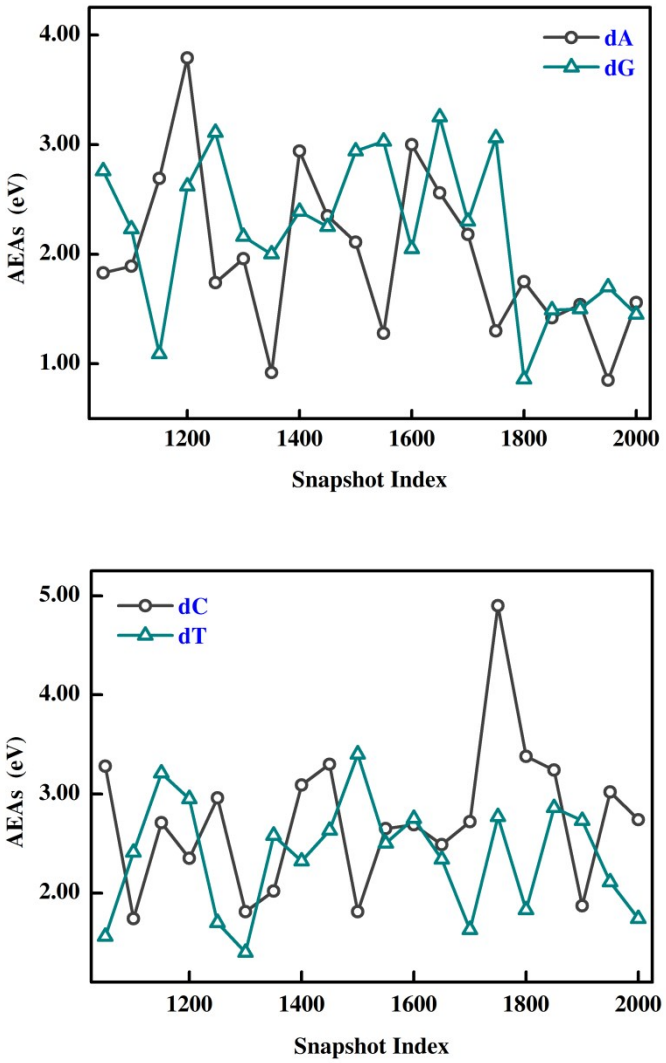

Figure S8. Vertical Detachment Energies (VDEs) of QM/MM Computations for 20 Snapshots.

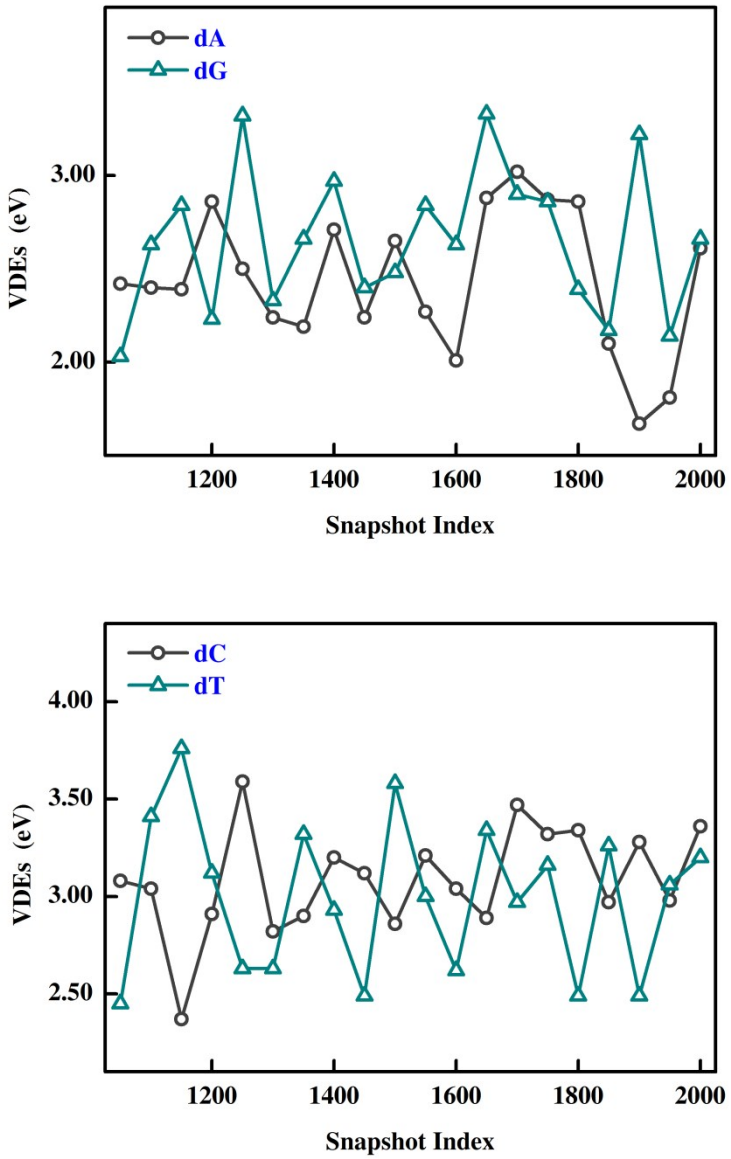

Table S1. Averaged numbers of atoms in QM regions of different sizes (R_{QM} in Å).

R_{QM}	dA	dG	dC	dT
1.6	**31**	**32**	**29**	**31**
1.8	**32**	**33**	**30**	**32**
2.0	**37**	**36**	**34**	**36**
2.2	**41**	**40**	**37**	**38**
2.4	**43**	**45**	**40**	**39**
2.6	**51**	**52**	**46**	**46**
2.8	**64**	**68**	**61**	**61**
3	**84**	**88**	**82**	**81**
3.2	**104**	**104**	**97**	**98**
3.4	**121**	**122**	**109**	**111**
3.6	**134**	**134**	**119**	**125**
3.8	**148**	**143**	**129**	**139**
4	**161**	**157**	**144**	**150**
4.2	**172**	**169**	**158**	**162**
4.4	**182**	**181**	**169**	**176**
4.6	**195**	**194**	**180**	**189**
4.8	**209**	**208**	**194**	**201**

Table S2. Standard errors (SEs) of VEA, AEA, and VDEs (eV).

	VEA		AEA			VDE	
	QM/MM	**gas-QM**	**QM/MM**	**pol-QM**	**gas-QM**	**QM/MM**	**gas-QM**
dA	**0.05**	**0.08**	**0.17**	**0.16**	**0.07**	**0.08**	**0.07**
dG	**0.05**	**0.06**	**0.16**	**0.21**	**0.08**	**0.09**	**0.09**
dC	**0.05**	**0.06**	**0.17**	**0.17**	**0.07**	**0.06**	**0.09**
dT	**0.06**	**0.06**	**0.13**	**0.16**	**0.08**	**0.09**	**0.08**

Table S3. Spin densities of anionic SP calculations at neutral and anionic optimized geometries.

	Neutral OPT		Anionic OPT	
	dRN	**bases**	**dRN**	**bases**
dA	**0.69**	**0.64**	**0.97**	**0.95**
dG	**0.60**	**0.53**	**0.94**	**0.87**
dC	**0.75**	**0.64**	**0.97**	**0.83**
dT	**0.82**	**0.71**	**0.98**	**0.86**