Electronic Supplementary Information for

Excess-electron Capture and Energy Transfer to Bulk Water for Aqueous DNA Nucleotide

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Table S1. Atomic number in QM region for each snapshot.

	$dAMP^-$	$dGMP^-$	$dCMP^-$	$dTMP^-$
1025	128	147	135	137
1050	125	144	138	140
1075	143	138	129	134
1100	140	135	138	143
1125	134	126	126	128
1150	140	135	123	143
1175	131	147	120	134
1200	146	147	120	152
1225	131	150	123	134
1250	134	135	129	131
1275	137	132	129	146
1300	125	144	129	137
1325	146	144	129	134
1350	125	126	126	149
1375	134	144	123	143
1400	131	126	141	146
1425	140	138	132	140
1450	134	147	132	143
1475	137	144	129	146
1500	134	144	132	143
1525	131	129	111	125
1550	134	132	138	152
1575	122	141	129	140
1600	122	141	129	140
1625	131	144	123	134
1650	143	144	138	134
1675	134	132	132	131
1700	152	141	129	146
1725	131	138	132	137
1750	125	132	120	137
1775	128	138	114	131
1800	143	147	138	128
1825	137	138	129	125
1850	140	147	150	128
1875	137	150	138	134
1900	146	153	138	146
1925	140	150	144	155
1950	140	135	129	122
1975	134	144	123	137
2000	149	132	138	134
Ave.	135	140	130	138

Table S2. Excess-electron distributions of pol-QM and gas-QM computations averaged over 40 snapshots in vertical electron attachment and standard errors (*e*).

	dAMP$^-$ → dAMP^{2-}	**dGMP$^-$ → dGMP^{2-}**	**dCMP$^-$ → dCMP^{2-}**	**dTMP$^-$ → dTMP^{2-}**
Q_{dRT}(gas-QM)	**–0.08 ± 0.02**	**–0.07 ± 0.01**	**–0.11 ± 0.02**	**–0.19 ± 0.03**
Q_{dRT}(pol-QM)	**–0.49 ± 0.02**	**–0.38 ± 0.02**	**–0.47 ± 0.02**	**–0.52 ± 0.02**
Q_{base}(pol-QM)	**–0.40 ± 0.02**	**–0.31 ± 0.02**	**–0.37 ± 0.02**	**–0.41 ± 0.02**
Q_{ribose}(pol-QM)	**–0.05 ± 0.01**	**–0.02 ± 0.01**	**–0.04 ± 0.01**	**–0.06 ± 0.01**

Table S3. Mean excess-electron distributions and standard errors in adiabatic electron attachment to aqueous dRT^- and standard errors (e).

	$dAMP^- \rightarrow dAMP^{2-}$	**$dGMP^- \rightarrow dGMP^{2-}$**	**$dCMP^- \rightarrow dCMP^{2-}$**	**$dTMP^- \rightarrow dTMP^{2-}$**
Q_{dRT}	**–0.84 ± 0.04**	**–0.78 ± 0.06**	**–0.89 ± 0.04**	**–0.91 ± 0.04**
Q_{base}	**–0.79 ± 0.04**	**–0.67 ± 0.06**	**–0.72 ± 0.04**	**–0.75 ± 0.04**
Q_{ribose}	**0.04 ± 0.04**	**–0.09 ± 0.05**	**–0.13 ± 0.04**	**–0.13 ± 0.04**

Table S4. Mean energy differences (eV) of dRT^{2-} between gas-QM and pol-QM calculations.

	$dAMP^{2-}$	**$dGMP^{2-}$**	**$dCMP^{2-}$**	**$dTMP^{2-}$**
$\Delta E^{2-}_{QM}(A)_a$	**37.08 ± 0.09**	**37.67 ± 0.09**	**36.95 ± 0.07**	**36.89 ± 0.11**
$\Delta E^{2-}_{QM}(B)_b$	**40.59 ± 0.11**	**41.46 ± 0.13**	**40.77 ± 0.10**	**40.19 ± 0.14**

[a] At optimized anionic structures. [b] At optimized dianionic structures.

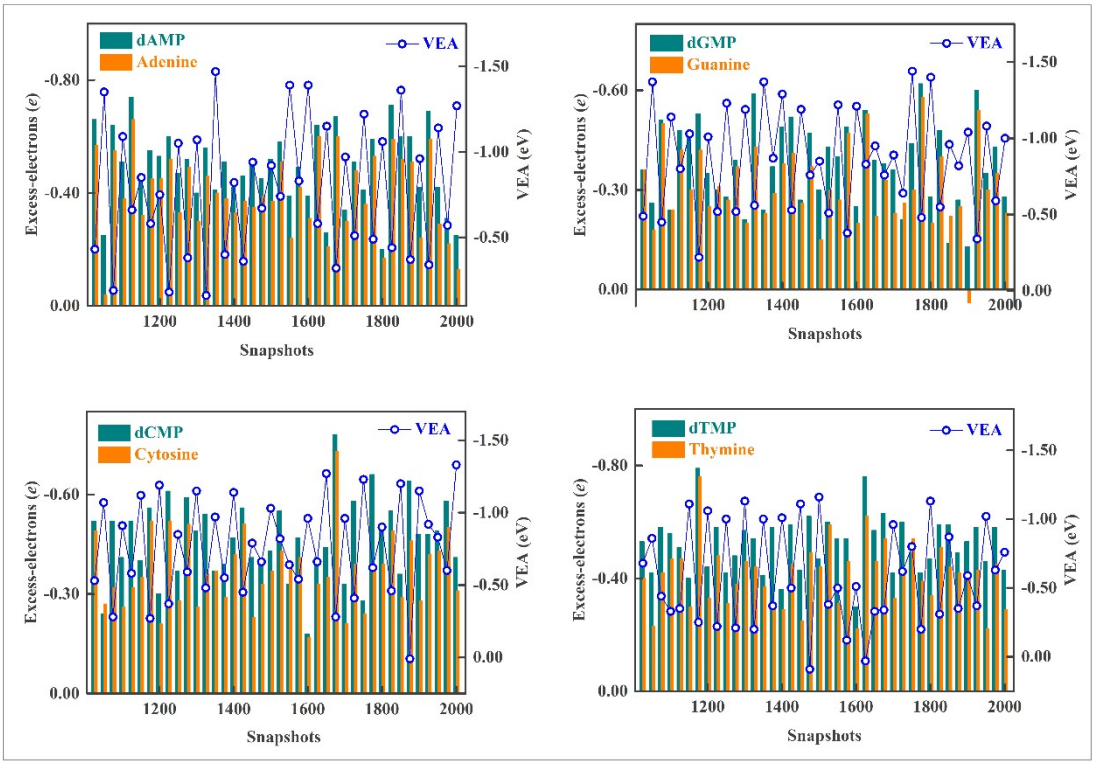

Figure S1. Excess-electron distributions in vertical excess-electron attachment to aqueous dRT^- and QM/MM VEAs for 40 snapshots.

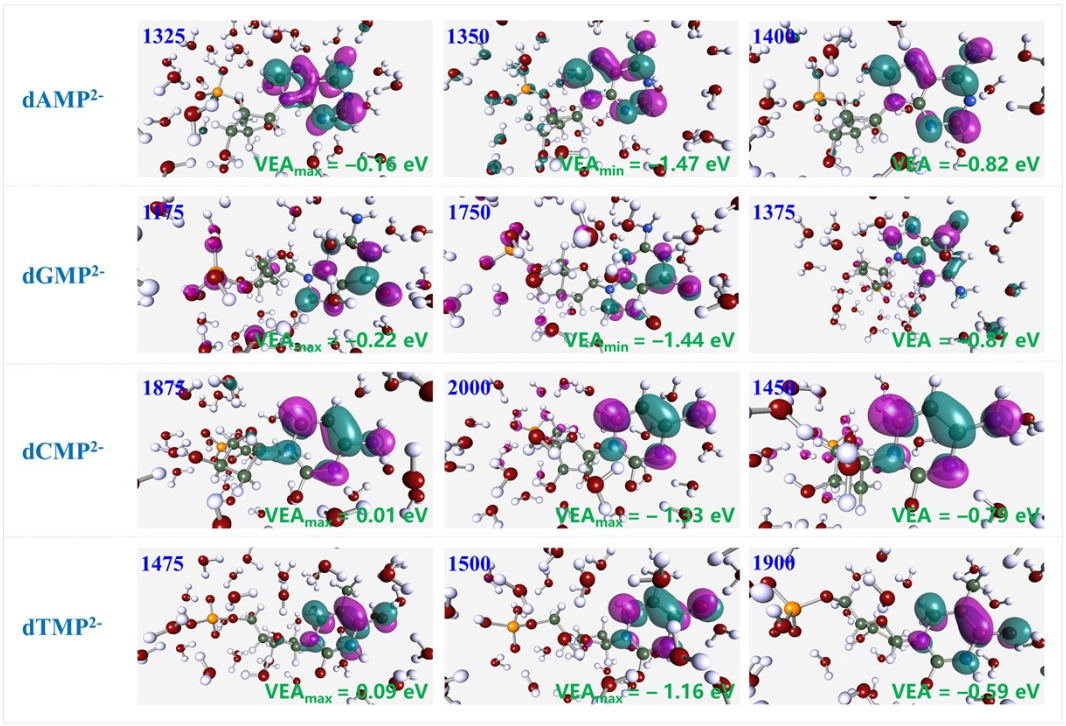

Figure S2. SOMOs of pol-QM calculation for representative snapshots at optimized anionic structures.

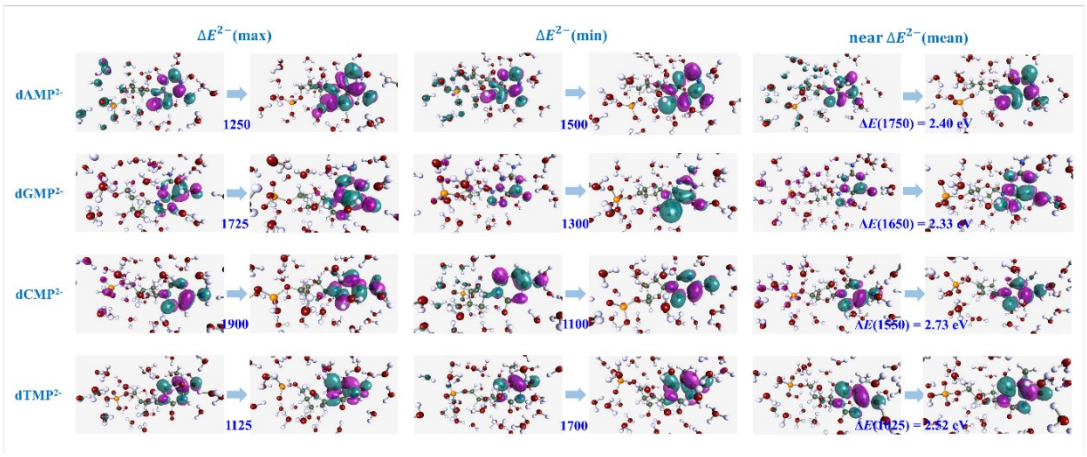

Figure S3. dRT^{2-} SOMOs of pol-QM calculations at optimized structures of anions and dianions for representative snapshots.