

Understanding the interaction of DNA-RNA Nucleobases with different ZnO Nanomaterials

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Table 1: Mulliken charge analysis (δq) for Guanine due to interaction with ZnO nanoparticles

	Isolated	With (ZnO) ₃ NW	With ZnO(10 $\bar{1}$ 0) surface	With ZnO(30,0) NT	With (ZnO) ₉₆ QD
O ₁	-0.511	-0.465	-0.489	-0.449	-0.438
N ₂	-0.469	-0.285	-0.278	-0.332	-0.336
N ₃	-0.244	-0.232	-0.222	-0.242	-0.239
N ₄	-0.288	-0.265	-0.300	-0.195	-0.172
N ₅	-0.087	-0.086	-0.062	-0.046	-0.046
N ₆	-0.364	-0.264	-0.240	-0.244	-0.212
C ₇	0.423	0.406	0.397	0.435	0.428
C ₈	0.486	0.491	0.493	0.509	0.509
C ₉	0.195	0.188	0.189	0.188	0.184
C ₁₀	-0.087	-0.059	-0.065	-0.078	-0.061
C ₁₁	0.058	0.111	0.099	0.114	0.129
H ₁₂	0.078	0.099	0.092	0.125	0.127
H ₁₃	0.197	0.272	0.223	0.240	0.235
H ₁₄	0.206	0.222	0.219	0.246	0.237
H ₁₅	0.193	0.197	0.200	0.214	0.217
H ₁₆	0.213	0.272	0.252	0.238	0.239
Total	0.000	0.602	0.508	0.723	0.801

Table 2: Mulliken charge analysis (δq) for Cytosine due to interaction with ZnO nanoparticles

	Isolated	With (ZnO) ₃ NW	With ZnO(10 $\bar{1}$ 0) surface	With ZnO(30,0) NT	With (ZnO) ₉₆ QD
O ₁	-0.557	-0.472	-0.511	-0.500	-0.445
N ₂	-0.469	-0.333	-0.379	-0.335	-0.388
N ₃	-0.161	-0.134	-0.178	-0.146	-0.173
N ₄	-0.326	-0.305	-0.211	-0.200	-0.267
C ₅	-0.303	-0.263	-0.335	-0.282	-0.328
C ₆	0.366	0.406	0.339	0.338	0.412
C ₇	0.073	0.075	0.196	0.115	0.168
C ₈	0.601	0.620	0.630	0.624	0.602
H ₉	0.207	0.229	0.247	0.242	0.238
H ₁₀	0.073	0.092	0.073	0.107	0.127
H ₁₁	0.092	0.109	0.125	0.118	0.124
H ₁₂	0.193	0.234	0.203	0.205	0.231
H ₁₃	0.211	0.233	0.223	0.226	0.236
Total	0.000	0.491	0.422	0.512	0.537

Table 3: Mulliken charge analysis (δq) for Thymine due to interaction with ZnO nanoparticles

	Isolated	With (ZnO) ₃ NW	With ZnO(10 $\bar{1}$ 0) surface	With ZnO(30,0) NT	With (ZnO) ₉₆ QD
O ₁	-0.554	-0.495	-0.496	-0.478	-0.463
O ₂	-0.496	-0.435	-0.438	-0.432	-0.408
N ₃	-0.185	-0.164	-0.164	-0.174	-0.122
N ₄	-0.262	-0.385	-0.382	-0.214	-0.206
C ₅	0.569	0.599	0.602	0.585	0.591
C ₆	0.486	0.521	0.524	0.499	0.493
C ₇	-0.001	0.00009	0.00047	0.009	-0.007
C ₈	-0.149	-0.138	-0.139	-0.129	-0.089
C ₉	-0.169	-0.175	-0.174	-0.175	-0.181
H ₁₀	0.083	0.081	0.078	0.102	0.087
H ₁₁	0.083	0.092	0.091	0.088	0.123
H ₁₂	0.058	0.059	0.056	0.065	0.081
H ₁₃	0.087	0.088	0.087	0.099	0.122
H ₁₄	0.232	0.327	0.319	0.266	0.252
H ₁₅	0.217	0.218	0.217	0.228	0.239
Total	0.000	0.193	0.181	0.339	0.512

Table 4: Mulliken charge analysis (δq) for Uracil due to interaction with ZnO nanoparticles

	Isolated	With (ZnO) ₃ NW	With ZnO(10 $\bar{1}$ 0) surface	With ZnO(30,0) NT	With (ZnO) ₉₆ QD
O ₁	-0.550	-0.493	-0.493	-0.479	-0.491
O ₂	-0.494	-0.433	-0.437	-0.412	-0.405
N ₃	-0.181	-0.163	-0.162	-0.166	-0.067
N ₄	-0.262	-0.385	-0.382	-0.215	-0.178
C ₅	0.573	0.603	0.606	0.589	0.595
C ₆	0.503	0.539	0.541	0.512	0.566
C ₇	0.044	0.044	0.044	0.063	0.193
C ₈	-0.287	-0.277	-0.278	-0.282	-0.228
H ₉	0.085	0.086	0.085	0.098	0.099
H ₁₀	0.119	0.119	0.114	0.130	0.121
H ₁₁	0.232	0.326	0.319	0.270	0.235
H ₁₂	0.218	0.219	0.218	0.229	0.225
Total	0.000	0.185	0.175	0.337	0.665