Describing the adsorption of doxorubicin on PAMAM dendrimer by *ab initio* calculations†

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Table SM 1 Calculated binding energy (E_1), G0 total energy calculated with the DOX ghost orbitals (A_{ghostB}), DOX total energy calculated with the G0 ghost orbitals (B_{ghostA}), G0 total energy (E(A)), DOX total energy (E(B)), and BSSE corrected binding energy (E_b) for all the interaction sites. The equation $E_b = E_1 - BSSE$, where $BSSE = A_{ghostB} + B_{ghostA} - E(A) - E(B)$ was used to obtain the corrected binding energies.

Site	E_1 (eV)	A_{ghostB} (eV)	B_{ghostA} (eV)	E(A) (eV)	E(B) (eV)	E_b (eV)
1	-0.75	-8929.627	-10039.670	-8929.567	-10039.607	-0.63
2	-0.61	-8929.505	-10039.615	-8929.484	-10039.593	-0.57
3	-0.71	-8929.585	-10039.633	-8929.537	-10039.612	-0.64
4	-0.65	-8929.513	-10039.562	-8929.508	-10039.564	-0.65
5	-0.75	-8929.632	-10039.662	-8929.532	-10039.593	-0.58
6	-0.73	-8929.723	-10039.753	-8929.476	-10039.604	-0.33
7	-0.71	-8929.490	-10039.713	-8929.469	-10039.607	-0.58
8	-0.74	-8929.602	-10039.683	-8929.520	-10039.609	-0.58
9	-1.16	-8929.711	-10039.619	-8929.532	-10039.459	-0.82
10	-0.91	-8929.561	-10039.743	-8929.523	-10039.611	-0.74
11	-0.71	-8929.546	-10039.798	-8929.505	-10039.591	-0.46

Table SM 2 Calculated binding energy (E_1), G0.NHAc.FA total energy calculated with the DOX ghost orbitals (A_{ghostB}), DOX total energy calculated with the G0.NHAc.FA ghost orbitals (B_{ghostA}), G0.NHAc.FA total energy (E(A)), DOX total energy (E(B)), and BSSE corrected binding energy (E_b) for all the interaction sites. The equation $E_b = E_1 - BSSE$, where $BSSE = A_{ghostB} + B_{ghostA} - E(A) - E(B)$ was used to obtain the corrected binding energies.

Site	E_1 (eV)	A_{ghostB} (eV)	B_{ghostA} (eV)	E(A) (eV)	E(B) (eV)	E_b (eV)
1	-0.72	-18086.729	-10039.648	-18086.734	-10039.592	-0.67
2	-0.66	-18086.720	-10039.671	-18086.695	-10039.601	-0.57
3	-0.74	-18086.729	-10039.590	-18086.775	-10039.609	-0.81
4	-0.71	-18086.606	-10039.674	-18086.707	-10039.609	-0.75
5	-0.80	-18086.765	-10039.681	-18086.773	-10039.592	-0.72
6	-0.73	-18086.741	-10039.697	-18086.711	-10039.584	-0.59
7	-0.96	-18086.919	-10039.668	-18086.793	-10039.562	-0.73
8	-0.86	-18086.729	-10039.497	-18086.763	-10039.501	-0.90
9	-1.37	-18086.884	-10039.493	-18086.769	-10039.360	-1.12
10	-0.86	-18086.773	-10039.608	-18086.731	-10039.550	-0.76
11	-0.80	-18086.717	-10039.686	-18086.642	-10039.568	-0.61

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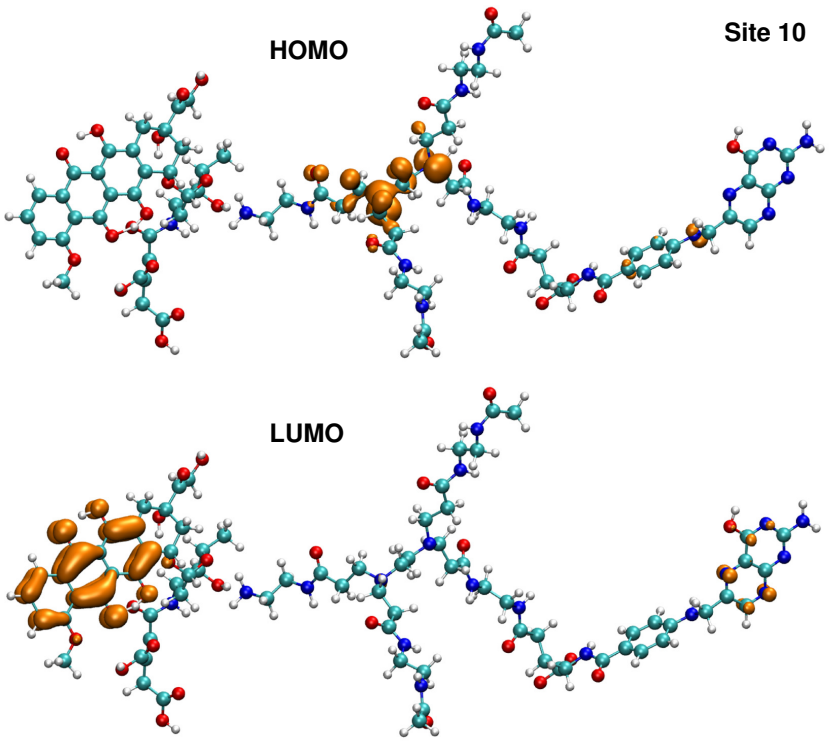
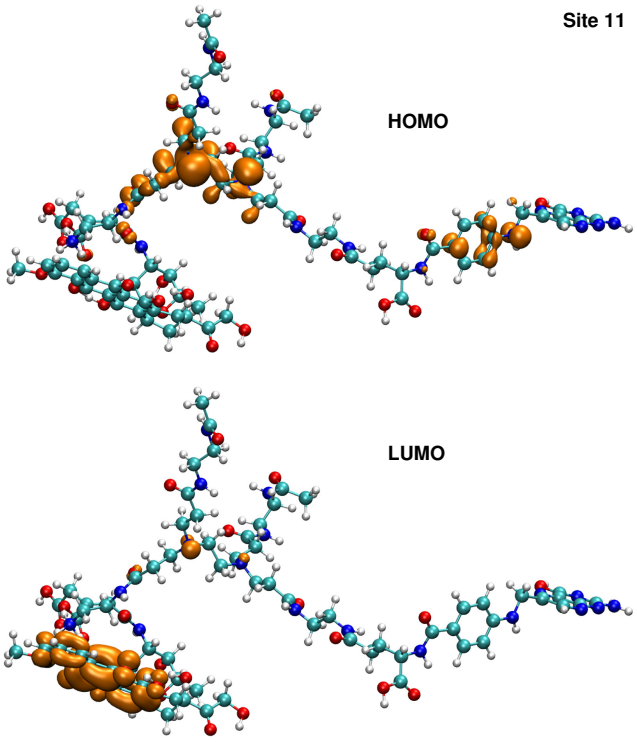
Table SM 3 Calculated binding energy (E_1), G0.NHAc.FA total energy calculated with the DOX.cis ghost orbitals (A_{ghostB}), DOX.cis total energy calculated with the G0.NHAc.FA ghost orbitals (B_{ghostA}), G0.NHAc.FA total energy (E(A)), DOX.cis total energy (E(B)), and BSSE corrected binding energy (E_b) for all the interaction sites. The equation $E_b = E_1 - BSSE$, where $BSSE = A_{ghostB} + B_{ghostA} - E(A) - E(B)$ was used to obtain the corrected binding energies.

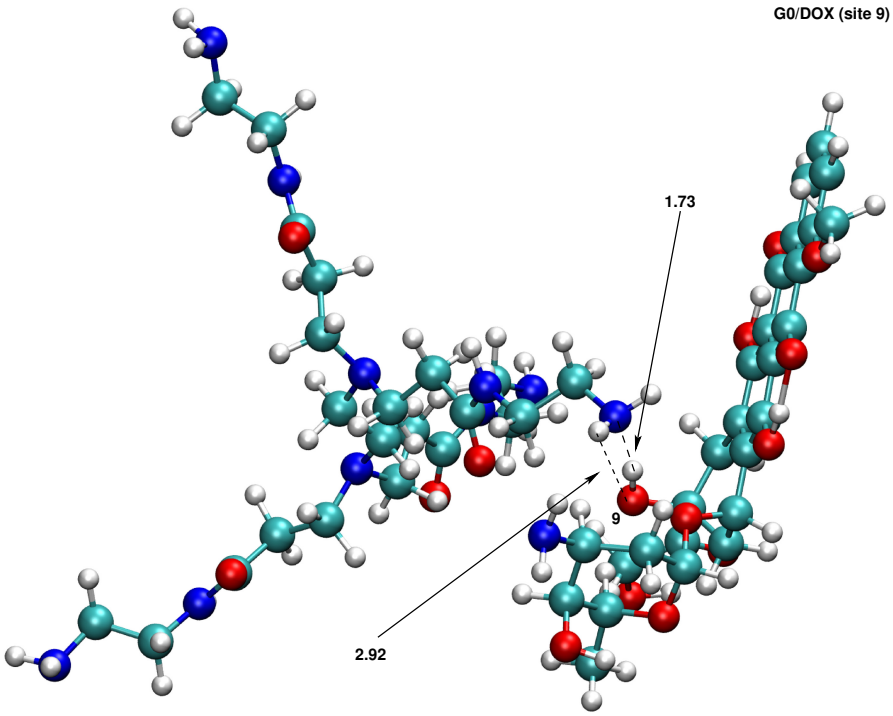
Site	E_1 (eV)	A_{ghostB} (eV)	B_{ghostA} (eV)	E(A) (eV)	E(B) (eV)	E_b (eV)
1	-0.70	-18086.750	-13310.894	-18086.712	-13310.780	-0.55
2	-0.86	-18086.830	-13310.902	-18086.832	-13310.864	-0.82
3	-0.79	-18086.794	-13310.851	-18086.807	-13310.807	-0.76
4	-1.07	-18086.792	-13310.944	-18086.727	-13310.752	-0.81
5	-1.19	-18086.626	-13311.132	-18086.659	-13310.659	-0.90
6	-0.77	-18086.728	-13310.920	-18086.654	-13310.786	-0.56
7	-0.98	-18087.029	-13310.936	-18086.927	-13310.795	-0.74
8	-0.94	-18086.899	-13310.825	-18086.835	-13310.821	-0.87
9	-1.24	-18086.852	-13310.919	-18086.631	-13310.646	-0.75
10	-0.84	-18086.600	-13310.749	-18086.569	-13310.620	-0.68
11	-1.60	-18086.826	-13310.806	-18086.593	-13310.427	-0.99



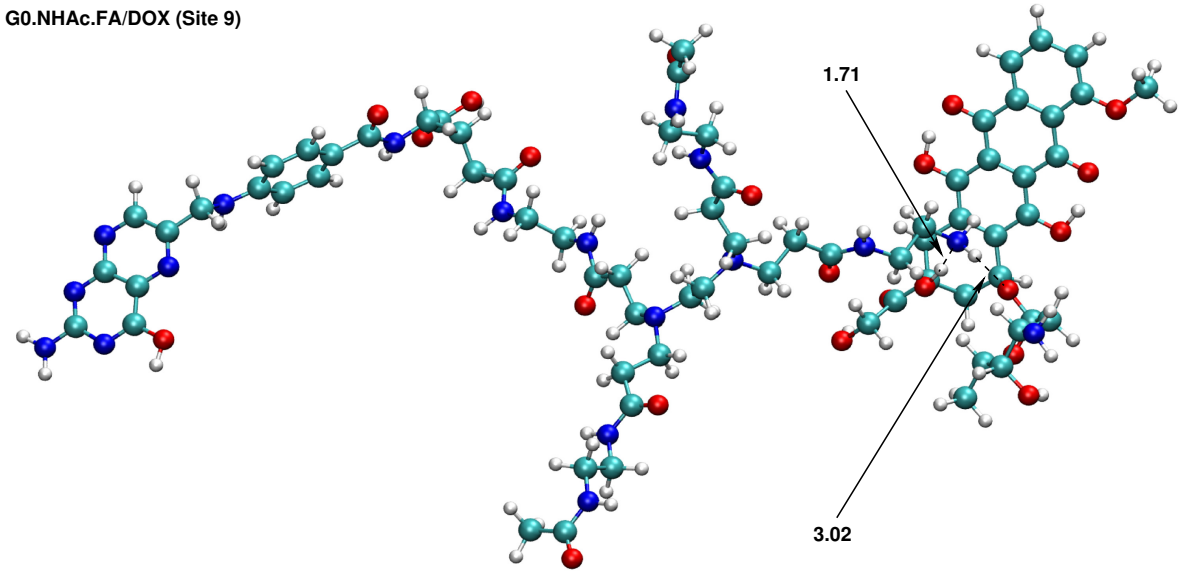
SM 1 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 10). The local density of states for the HOMO and LUMO levels is represented in orange. The colors of the atoms are cyan for C, red for O, blue for N, and white for H.



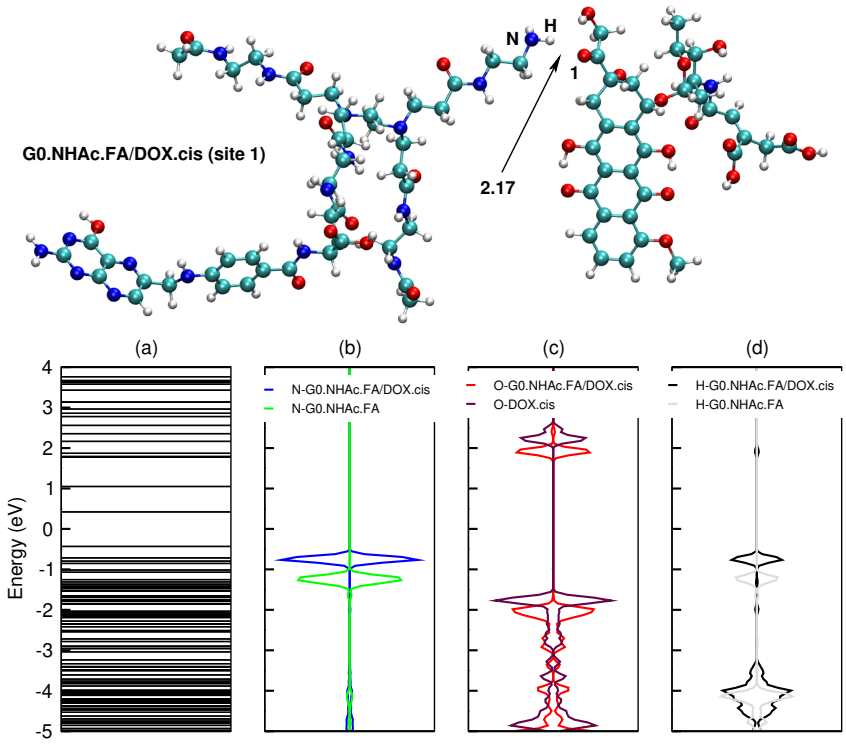
SM 2 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 11). The local density of states for the HOMO and LUMO levels is represented in orange. The colors of the atoms are cyan for C, red for O, blue for N, and white for H.



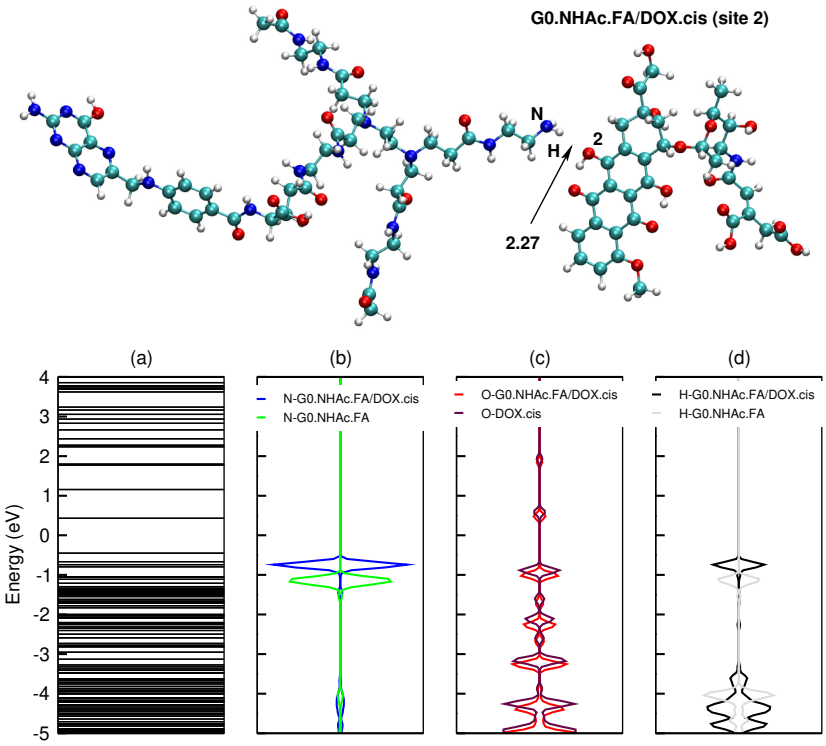
SM 3 Full relaxed geometry for the G0/DOX.cis (Site 9). The colors of the atoms are cyan for C, red for O, blue for N, and white for H.



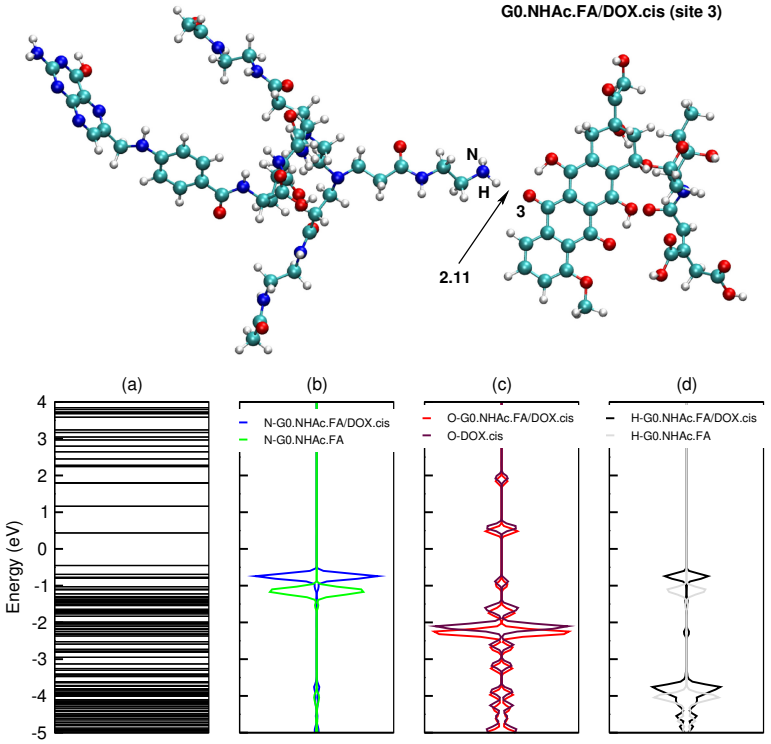
SM 4 Full relaxed geometry for the G0.NHAc.FA/DOX (Site 9). The colors of the atoms are cyan for C, red for O, blue for N, and white for H.



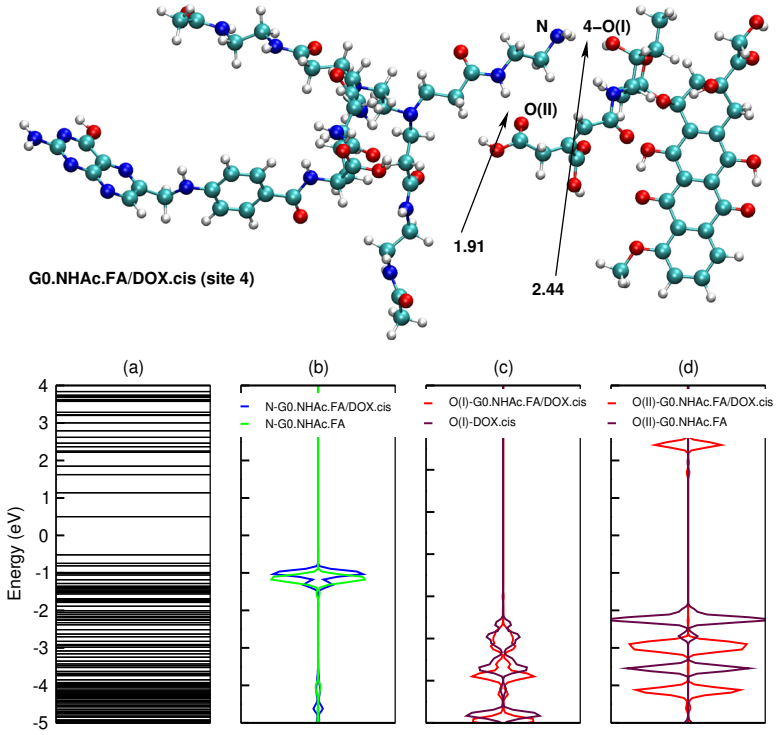
SM 5 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 1). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



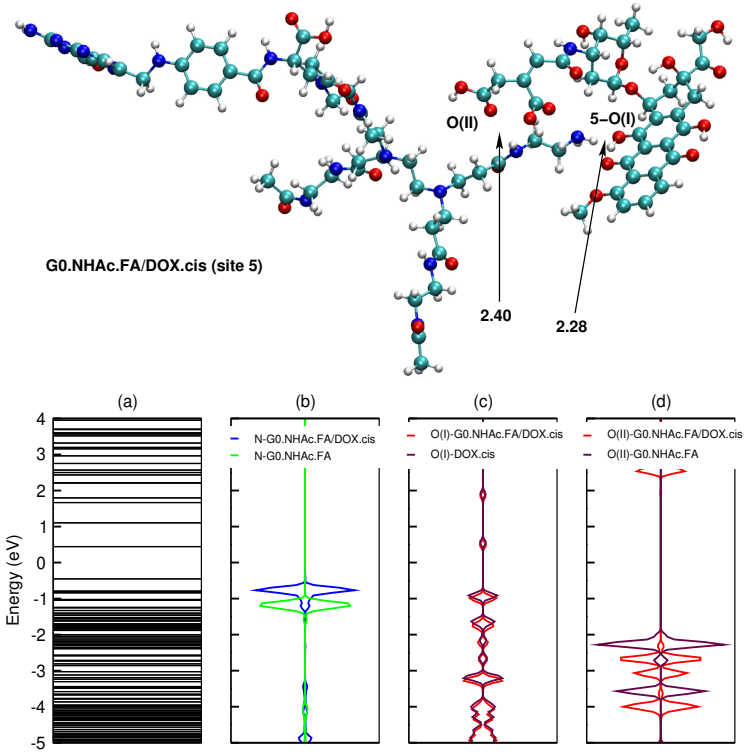
SM 6 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 2). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



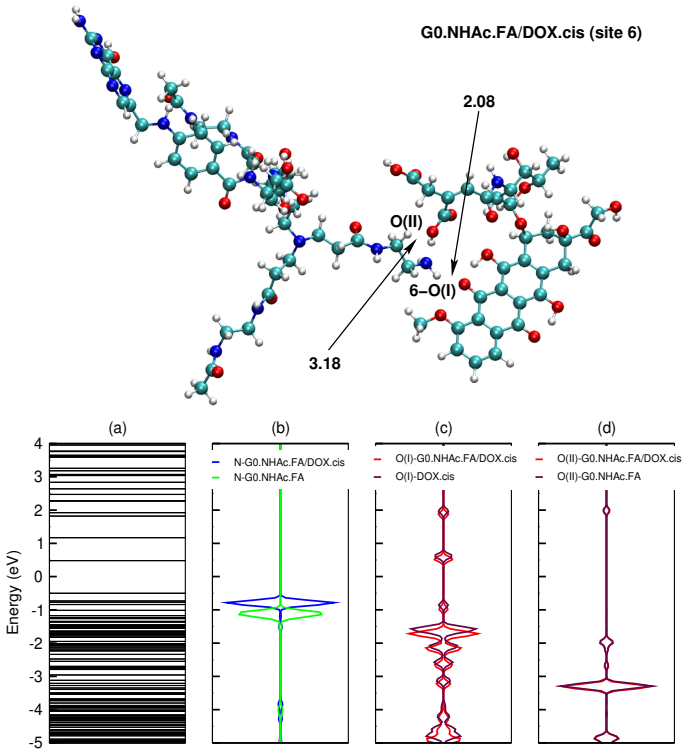
SM 7 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 3). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



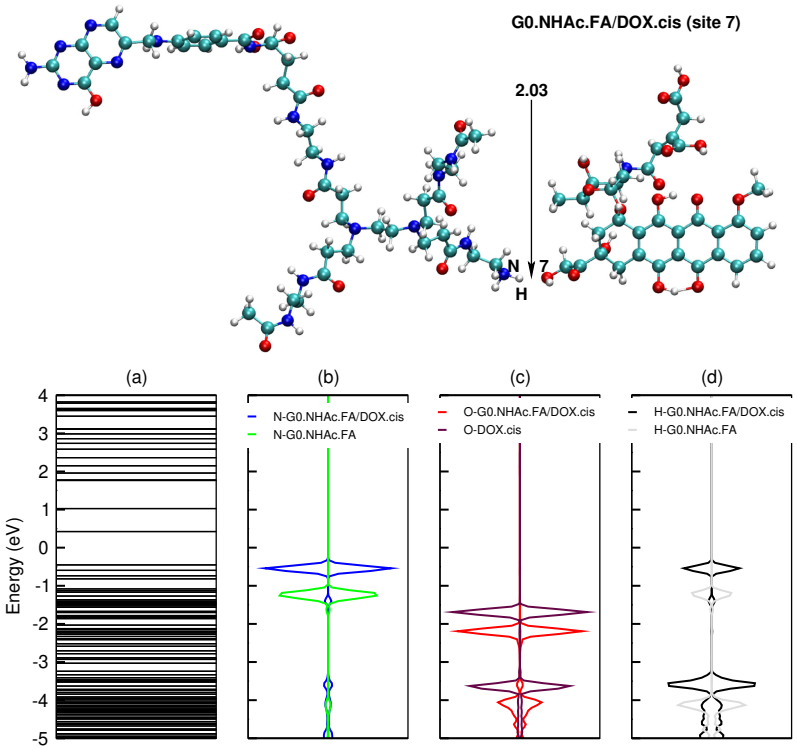
SM 8 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 4). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



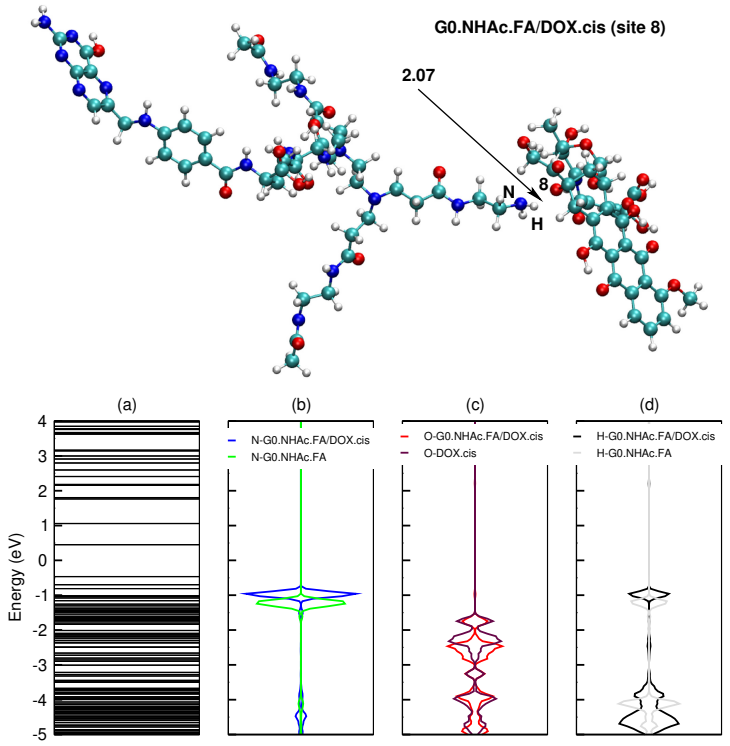
SM 9 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 5). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



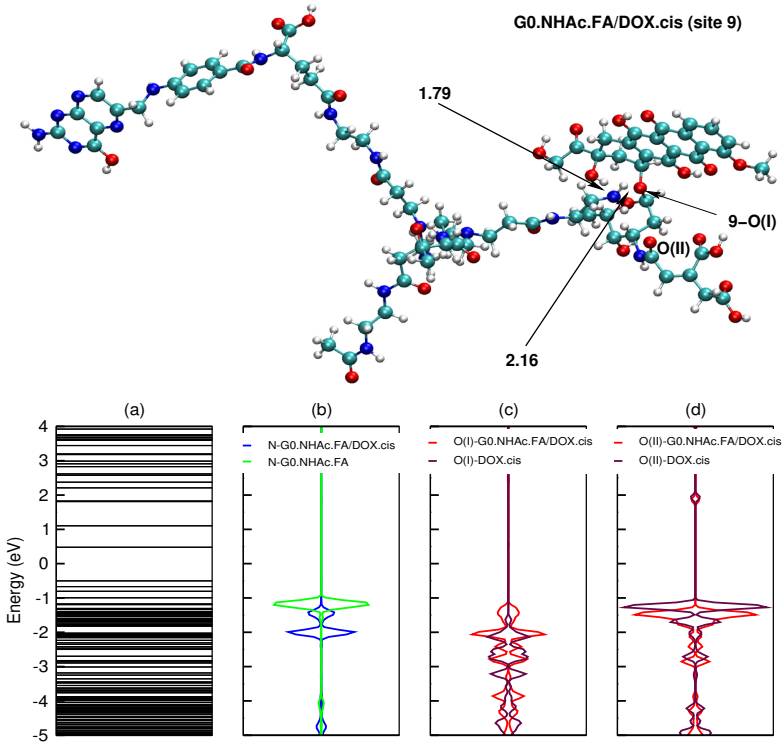
SM 10 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 6). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



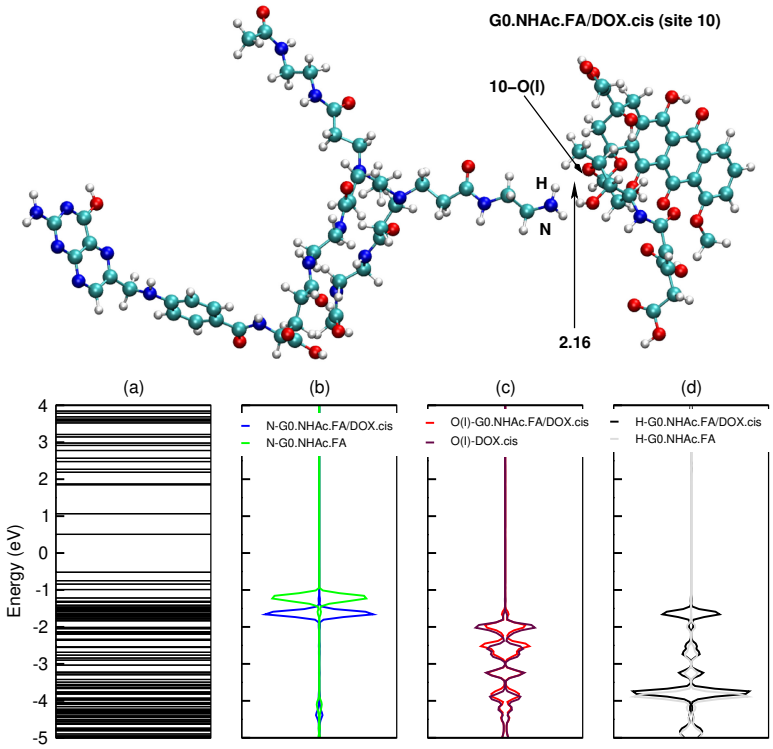
SM 11 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 7). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



SM 12 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 8). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



SM 13 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 9). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.



SM 14 Full relaxed geometry for the G0.NHAc.FA/DOX.cis (Site 10). The colors of the atoms are cyan for C, red for O, blue for N, and white for H. In (a) the energy levels are represented. In (b)-(d) the pDOS on chosen atoms are showed. For all figures the Fermi level is set to zero.