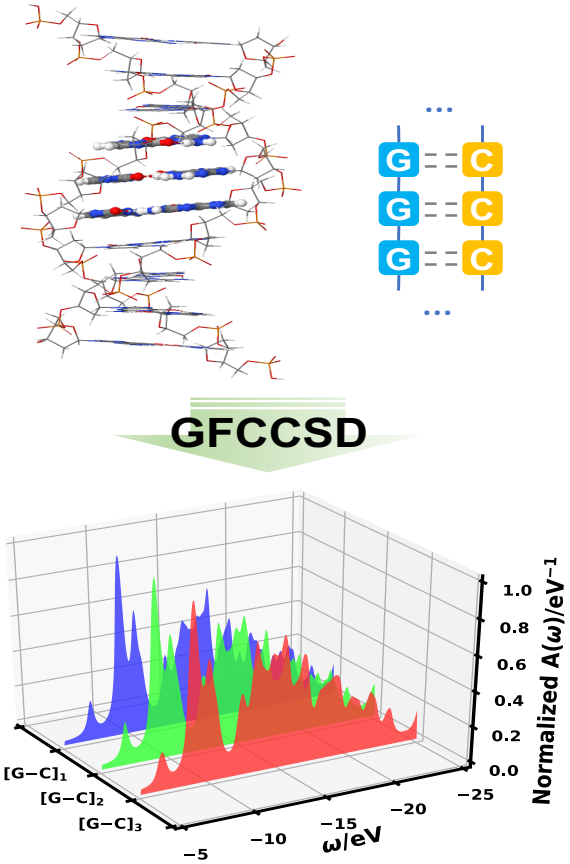
The Near Valence Ionization of DNA Fragments



Upper: Schematic of G-C stacked structures

Lower: Spectral functions of G-C base pairs, $[G\text{-}C]_n$ (n=1-3), in the [-25,-5] eV near-valence energy regime computed at the GFCCSD/6-31++G(d) level

Bo Peng, Karol Kowalski, Ajay Panyala, Sriram Krishnamoorthy, *J. Chem. Phys.* **152**, 011101 (2020)

Scientific Achievement

This study reveals the importance of two-body interactions in the near valence ionization of large DNA fragments

Significance and Impact

The ionization of large DNA fragments have for the first time been simulated with the many-body Green's function coupled cluster method over a broad valence energy regime. The inclusion of two-body components (two holes, one particle) reveals an important transition from intra- to inter-base-pair excitation as we increase the fragment size.

Research Details

- The spectral functions of up to three guanine-cytosine [G-C] base pairs have been computed in the range from [-25.0,-5.0] eV using SPEC's Green's function coupled cluster with single and double (GFCCSD) library on the *Summit* supercomputer
- As the fragment size increases, the lowest valence ionization energies decrease, but the relative peak positions do not change.
- The inter-base-pair excitation must include at least two base pairs in the quantum region for this transition to become apparent.

Work was performed at Pacific Northwest National Laboratory

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