Tunable Crystallinity and Charge Transfer in Two-Dimensional G-Quadruplex Organic Frameworks

Scientific Achievement

G-quadruplex organic frameworks (3D guanine structures found in DNA) were tuned with 2,7-diaryl pyrene and naphthalene diimide to study their structural and electronic properties: framework formation and photophysical properties were elucidated.

Significance and Impact

Decreasing the planarity of the building blocks helps to form 2D metal organic frameworks, which was applied here to form frameworks with G-quadruplex. The combination of the large optical gap and high lying HOMO energy of these materials implies applications as strong photoreductants for photocatalytic reactions.

Research Details

Tuned GQFs were synthesized and analyzed: $G_2\text{PhPyr}$, $G_2\text{TolPyr}$, $G_2\text{pXyPyr}$, and $G_2\text{mXyPyr}$ were confirmed by $^1\text{H}$ NMR and PXRD.

- Hypothetical structures were constructed using the Crystal Builder and Forcite modules of Materials Studio.
- Structural details were described by the computed interaction energy between the two G-quartet layers.