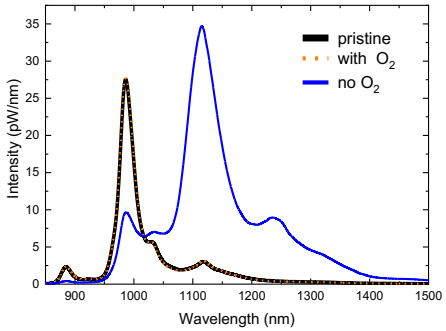
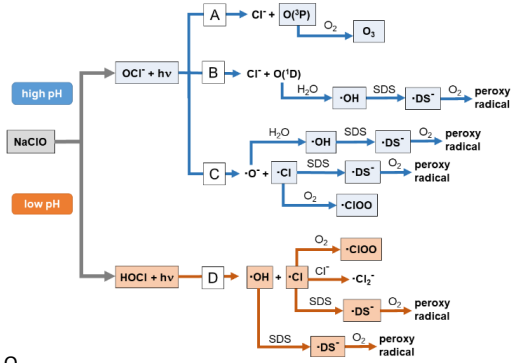
Complexity in the Photofunctionalization of Single-Wall Carbon Nanotubes with Hypochlorite

Scientific Achievement

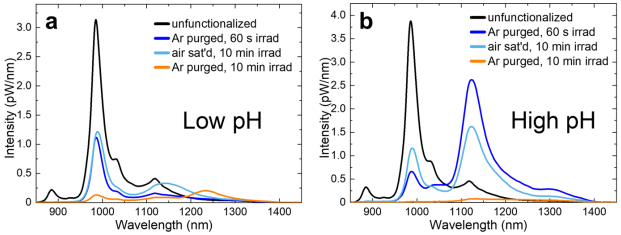
Exploration of the photofunctionalization of SWCNTs by NaClO at varying pH and dissolved oxygen levels reveals that the process is much more complex than previously realized.



Fluorescence spectra of products following HOCl photofunctionalization treatment show that dissolved O_2 strongly hinders the functionalization reaction.



Proposed relevant reaction pathways for photodissociation of NaOCl under low and high pH conditions



These spectra compare spectra of products formed under low and high pH reaction conditions. While similarities suggest similar exciton trap depths, study results show that different pH levels lead to different chemical adducts.

Significance and Impact

- Prior reports claimed that nanotube photofunctionalization with NaClO gave oxygen doping through an addition reaction with O(^{1}D).
- This work reveals a different and more complex reaction process that depends strongly on sample conditions.
- This system can lead not only to O-doped SWCNTs, but also to adducts from addition of $^{\bullet}$OH and $^{\bullet}$Cl radicals.

Research Details

- Sodium hypochlorite was photolyzed by UV light in the presence of coated SWCNTs under both low and high pH conditions (giving initially HOCl and OCl$^-$) air-saturated and argon-saturated conditions.
- Resulting covalently functionalized SWCNTs were characterized with NIR fluorescence, UV-Vis absorption, and X-ray photoelectron Spectroscopies

This work was performed in part at The Center for Integrated Nanotechnologies.

Espinoza, V. B.; Bachilo, S. M.; Zheng, Y.; Htoon, H.; Weisman, R. B. Complexity in the Photofunctionalization of Single-Wall Carbon Nanotubes with Hypochlorite. *ACS Nano* **2025**, *19* (2), 2497–2506.

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