Nanowires in carbon nanotubes have huge solar energy applications

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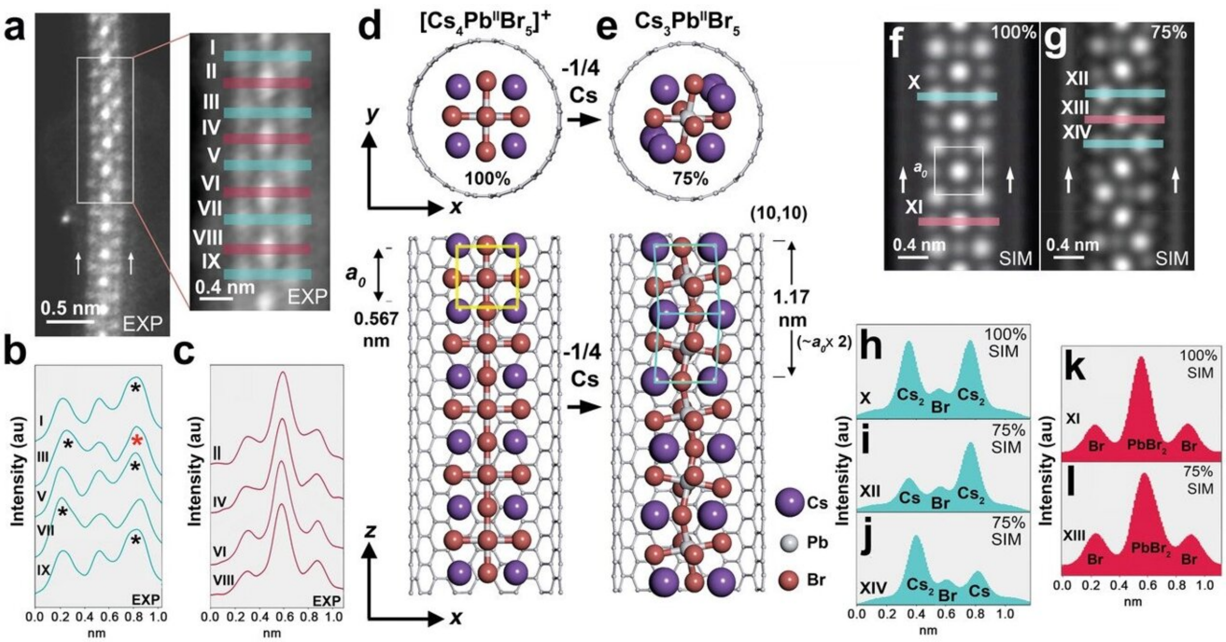

Encapsulated single-unit-cell wide $Cs_3Pb^{II}Br_5$ halide perovskite structure derived from $CsPbBr_3$. a) HAADF image of Cs_xPbBr_5 nanowire imaged inside a ≈1.4 nm SWCNT, walls indicated by arrows. Enlarged detail with 15 pixel wide regions indicated (I-X). b,c) Profiles I, III, V, VII, and IX from Cs_x–Br–$Cs_{x'}$ (x,x′ = 1 or 2) layers and II, IV, VI, and VIII from Br–$PbBr_2$–Br layers. Alternating Cs_2 columns in Cs_x–Br–$Cs_{x'}$ layers indicated by black asterisks with one excess Cs_2 column (red asterisk) indicated. d) DFT optimized $[Cs_4PbBr_5]^+$ nanowire (100% Cs occupancy) in a (10,10) SWCNT viewed end-on and side-on with the ABX_3 unit cell overlaid. e) DFT optimized $Cs_3Pb^{II}Br_5$ nanowire (75% Cs occupancy) formed by removing one-fourth of Cs atoms. This lowest energy form (Figure S3a-c, Supporting Information) has alternating Cs_2 columns and systematic $PbBr_6$ octahedral tilting. f,g) TDS STEM simulations of optimized

$[Cs_4Pb^{II}Br_5]^+$ and $Cs_3Pb^{II}Br_5$ structures. h,l) Simulated line profiles through Cs_x–Br–$Cs_{x'}$ and Br-$PbBr_2$–Br layers as indicated in (f) and (g). Credit: *Advanced Materials* (2022). DOI: 10.1002/adma.202208575

Tiny materials one hundred thousand times smaller than the width of a strand of hair could be used to improve solar cell technology.

A study published this month in *Advanced Materials* shows that materials as small as 1.2 nanometers across could function in solar cells, which harvest energy from the sun. The inorganic halide materials are templated within carbon nanotubes, tiny tubules formed from carbon atoms.

The discovery of such small nanowires could potentially lead to new properties and applications of this type of sustainable energy.

Researchers from the University of Warwick, Oxford Materials and SuperSTEM, a U.K. national center for electron microscopy, revealed the absolute minimum limit at which halide perovskite-like structures can be produced as free-standing materials inside carbon nanotube. Halide perovskites have similar structures to calcium titanate and are commonly used in solar panels and light emitting diodes (LEDs).

Dr. Jeremy Sloan, from Warwick's Department of Physics said, "In contrast to large 'bulk' halide perovskites, we show that much smaller 'picoscale' halide perovskite structures just a single unit cell or even just one quarter of a unit cell in cross section can be encapsulated in carbon nanotubes ranging between 1.2–1.6nm in diameter.

"Our study shows remarkably similar results to a publication in *Journal of the American Chemical Society (JACS)* by researchers at the University of Berkeley, further highlighting the potential applications of these tiny materials in solar cells.

"The wider implications of these studies will help to extend the remarkable optoelectronic characteristics of halide perovskites to sub-nanometer, or even picoscale dimensions."

More information: Reza J. Kashtiban et al, Picoperovskites: The Smallest Conceivable Isolated Halide Perovskite Structures Formed within Carbon Nanotubes, *Advanced Materials* (2022). [DOI: 10.1002/adma.202208575](https://dx.doi.org/10.1002/adma.202208575)

Provided by University of Warwick

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