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Reporting Summary

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Statistics

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.

n/a Confirmed

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|-------------------------------------|-------------------------------------|--|
| ☐ | ☒ | The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement |
| ☐ | ☒ | A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly |
| ☒ | ☐ | The statistical test(s) used AND whether they are one- or two-sided
<i>Only common tests should be described solely by name; describe more complex techniques in the Methods section.</i> |
| ☒ | ☐ | A description of all covariates tested |
| ☒ | ☐ | A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons |
| ☒ | ☐ | A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals) |
| ☒ | ☐ | For null hypothesis testing, the test statistic (e.g. F , t , r) with confidence intervals, effect sizes, degrees of freedom and P value noted
<i>Give P values as exact values whenever suitable.</i> |
| ☒ | ☐ | For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings |
| ☒ | ☐ | For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes |
| ☒ | ☐ | Estimates of effect sizes (e.g. Cohen's d , Pearson's r), indicating how they were calculated |

Our web collection on [statistics for biologists](#) contains articles on many of the points above.

Software and code

Policy information about [availability of computer code](#)

Data collection

All quantum-chemical calculations, molecular dynamics simulations, visualization, and symmetry analyses in this work were performed using the following software packages: VASP (6.3.1 04May22), Gaussian16 (C.01), LAMMPS (15Apr2020), OpenMolcas (23.10), VMD (1.9.3), Atomic Simulation Environment (ASE) package, cosymlib (v0.10.5)

Data analysis

Data analysis was carried out using Python (3.10.12) scripts together with the NumPy (2.2.5) and scikit-learn (1.6.1) libraries.

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Portfolio [guidelines for submitting code & software](#) for further information.

Data

Policy information about [availability of data](#)

All manuscripts must include a [data availability statement](#). This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A description of any restrictions on data availability
- For clinical datasets or third party data, please ensure that the statement adheres to our [policy](#)

The raw data used to generate the figures in this article have been summarized in an Excel file. Supplementary data associated with this paper, including the atomic coordinates of the structures, intermediate data from the fitting procedures, and the ReaxFF force-field parameters, will be uploaded.

Research involving human participants, their data, or biological material

Policy information about studies with [human participants or human data](#). See also policy information about [sex, gender \(identity/presentation\), and sexual orientation](#) and [race, ethnicity and racism](#).

Reporting on sex and gender

Reporting on race, ethnicity, or other socially relevant groupings

Population characteristics

Recruitment

Ethics oversight

Note that full information on the approval of the study protocol must also be provided in the manuscript.

Field-specific reporting

Please select the one below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.

☐ Life sciences ☐ Behavioural & social sciences ☒ Ecological, evolutionary & environmental sciences

For a reference copy of the document with all sections, see nature.com/documents/nr-reporting-summary-flat.pdf

Ecological, evolutionary & environmental sciences study design

All studies must disclose on these points even when the disclosure is negative.

Study description	This study investigated one-dimensional rare-earth chloride nanowires confined within single-walled carbon nanotubes, denoted LnCl ₃ @SWCNTs (Ln = Y, Gd, Dy, and Er). The work combined experimental characterization and theoretical modelling to resolve the local atomic structures and to correlate them with electronic and magnetic properties. The study was not designed as a factorial, nested, hierarchical, or other statistically comparative experiment. Rather, it was a materials synthesis and characterization study in which independently prepared material samples were analysed using commercial instruments and complementary computational methods. Experimental units consisted of independently prepared batches of LnCl ₃ @SWCNT materials for each lanthanide composition.
Research sample	The research samples were hybrid nanomaterials consisting of commercially available rare-earth chlorides (YCl ₃ , GdCl ₃ , DyCl ₃ , and ErCl ₃) encapsulated within commercially available single-walled carbon nanotubes. These materials were chosen because confinement inside SWCNTs can stabilize ordered one-dimensional structures and thereby enable investigation of structure–property relationships in low-dimensional rare-earth systems. The samples are intended to represent confined rare-earth chloride nanowires formed inside SWCNT hosts under the applied synthesis conditions. No biological organisms, human participants, sex, age range, or population-based sampling were involved in this study.
Sampling strategy	No formal statistical method was used to predetermine sample size, because this was not a hypothesis-testing study based on population inference. Instead, sample sizes were chosen according to standard practice in materials chemistry and condensed-matter experiments. For each composition, 3–4 independent sample preparations were carried out to provide sufficient material for the required characterizations. Because magnetic and electrical measurements were time-intensive and required pooling of material from multiple preparations to obtain sufficient sample quantity, these measurements were performed on combined samples. The chosen sample amounts were considered sufficient for obtaining the structural, spectroscopic, magnetic, and electronic data required for this study.
Data collection	All experimental data were collected by the authors using commercial instruments. Data acquisition and recording were performed automatically by the instrument control software, with no manual transcription involved; the resulting data were saved to the hard drive as binary or ASCII files. The characterization methods included TEM/STEM, thermogravimetric analysis (TGA), MPMS, PPMS, XPS, XAFS, and Raman spectroscopy. Computational data were generated using density functional theory (DFT), molecular dynamics (MD), and complete active space self-consistent field (CASSCF) calculations. Experimental data were collected between 2017 and 2018. Computational data were generated between 2024 and 2025. Instrumental outputs were recorded directly from the corresponding measurement systems and analysed by the authors.
Timing and spatial scale	Experimental data collection was conducted between 2017 and 2018, and computational analyses were conducted between 2024 and 2025. Measurements were acquired at multiple spatial scales depending on the technique, including local atomic- and nanoscale structural information from TEM/STEM and ensemble-averaged spectroscopic, magnetic, and electronic information from XPS, XAFS, Raman spectroscopy, MPMS, and PPMS. The timing and frequency of measurements were determined by sample preparation, instrument availability, and the need to obtain complementary structural and property data for each material system, rather than by a fixed sampling schedule. For each sample, the approximate measurement time was 3 h for TEM/STEM, 100 h for MPMS and PPMS measurements, and 1 h for XPS, XAFS, and Raman spectroscopy. No separate sample cohorts or defined gaps between collection periods were involved.

Data exclusions	No data were excluded from the analyses.
Reproducibility	Reproducibility of the experimental findings was verified by repeated sample preparation and repeated characterization where feasible. For each composition, 3–4 independent syntheses were performed to obtain sufficient material for characterization and to confirm synthetic reproducibility. All repeated synthesis attempts were successful. For structural and spectroscopic characterization, including TEM/STEM, TGA, XPS, XAFS, and Raman spectroscopy, consistent observations were obtained from samples prepared under the same synthesis conditions. Magnetic and electrical measurements using MPMS and PPMS were performed on pooled material from successful syntheses because these measurements required larger sample quantities and were time-intensive. All attempts to repeat the experimental measurements were successful, and no failed repeated experiments were observed.
Randomization	Randomization was not relevant to this study because the experiments did not involve the allocation of subjects, samples, treatments, or experimental units to different intervention groups. Instead, the study focused on the synthesis and instrumental characterization of material samples prepared under defined chemical conditions. Each sample composition and measurement condition was deliberately selected according to the material system under investigation, rather than randomly assigned. For the structural, spectroscopic, magnetic, and electrical measurements, the objective was to determine the intrinsic properties of each synthesized material under specified conditions. Randomizing samples or measurement conditions would therefore not be meaningful, because the measured signals originate from the physical and chemical characteristics of the materials themselves. Moreover, the experimentally synthesized materials are inherently mixed structures composed of Avogadro-scale numbers of molecular nanostructures, so the measured data represent ensemble-averaged properties, including contributions from any coexisting microscopic states within the sample. Therefore, randomization was not applied, as there were no randomized experimental groups or allocation procedures relevant to the study design.
Blinding	Blinding was not relevant to this study. Data acquisition was based on direct instrumental measurements of material samples, and no subjective outcome scoring or observer-dependent group assignment was involved during data collection or analysis.

Did the study involve field work? ☐ Yes ☒ No

Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

Materials & experimental systems

n/a	Involved in the study
☒	☐ Antibodies
☒	☐ Eukaryotic cell lines
☒	☐ Palaeontology and archaeology
☒	☐ Animals and other organisms
☒	☐ Clinical data
☒	☐ Dual use research of concern
☒	☐ Plants

Methods

n/a	Involved in the study
☒	☐ ChIP-seq
☒	☐ Flow cytometry
☒	☐ MRI-based neuroimaging

Plants

Seed stocks	No plants were involved in this study.
Novel plant genotypes	No plants were involved in this study.
Authentication	No plants were involved in this study.