



CURIE: Evaluating LLMs On Multitask Scientific Long Context Understanding and Reasoning





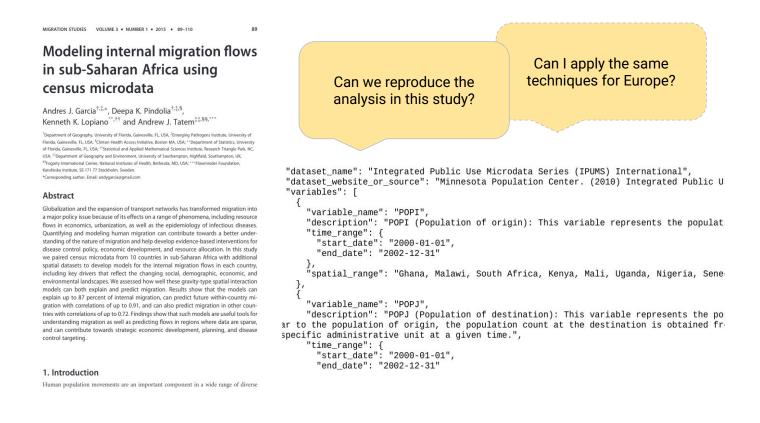
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Can LLMs assist Scientists with some workflows?

Can we measure problem solving ability?

- Extract details of the data.
- Identify and extract the processes and methodology.
- Write code to solve problem or reproduce study.

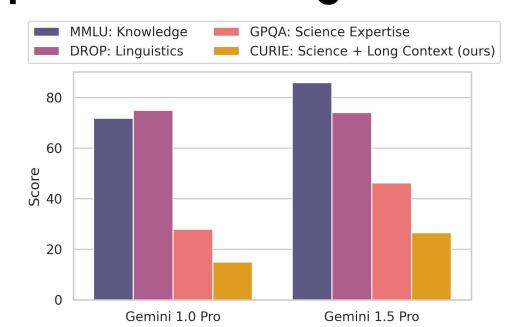


This requires

- Knowledge of the domain.I
- Processing long-context info.
- Reasoning ability to apply knowledge in the context of a problem.

CURIE: Tests scientific problem solving

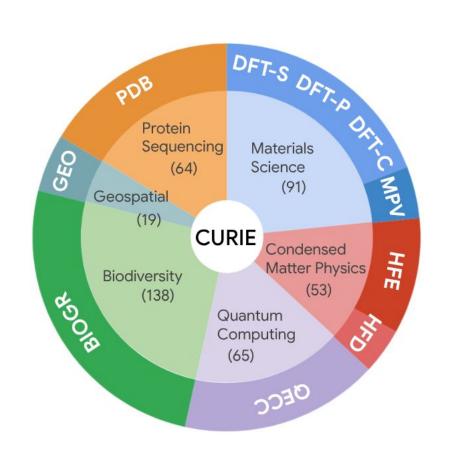
- Existing benchmarks test for knowledge, linguistics.
- CURIE: scientific long-Context Understanding Reasoning and Information Extraction benchmark

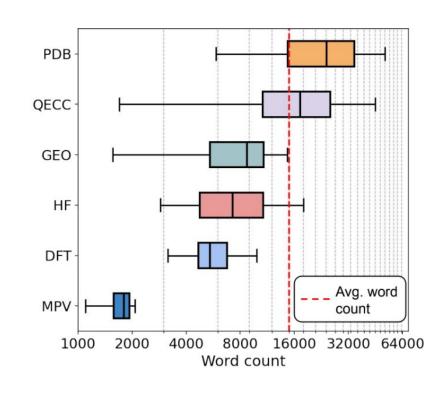


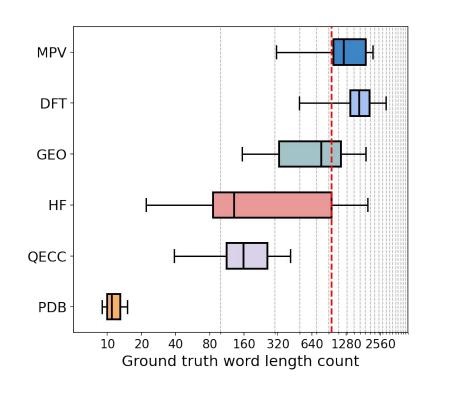
The CURIE benchmark and dataset

580 examples, 429 documents, 10 tasks, 6 domains

- Tasks require expertise + reasoning + long-context understanding
- Avg. input query length ~15k words, gold response length is ~1k





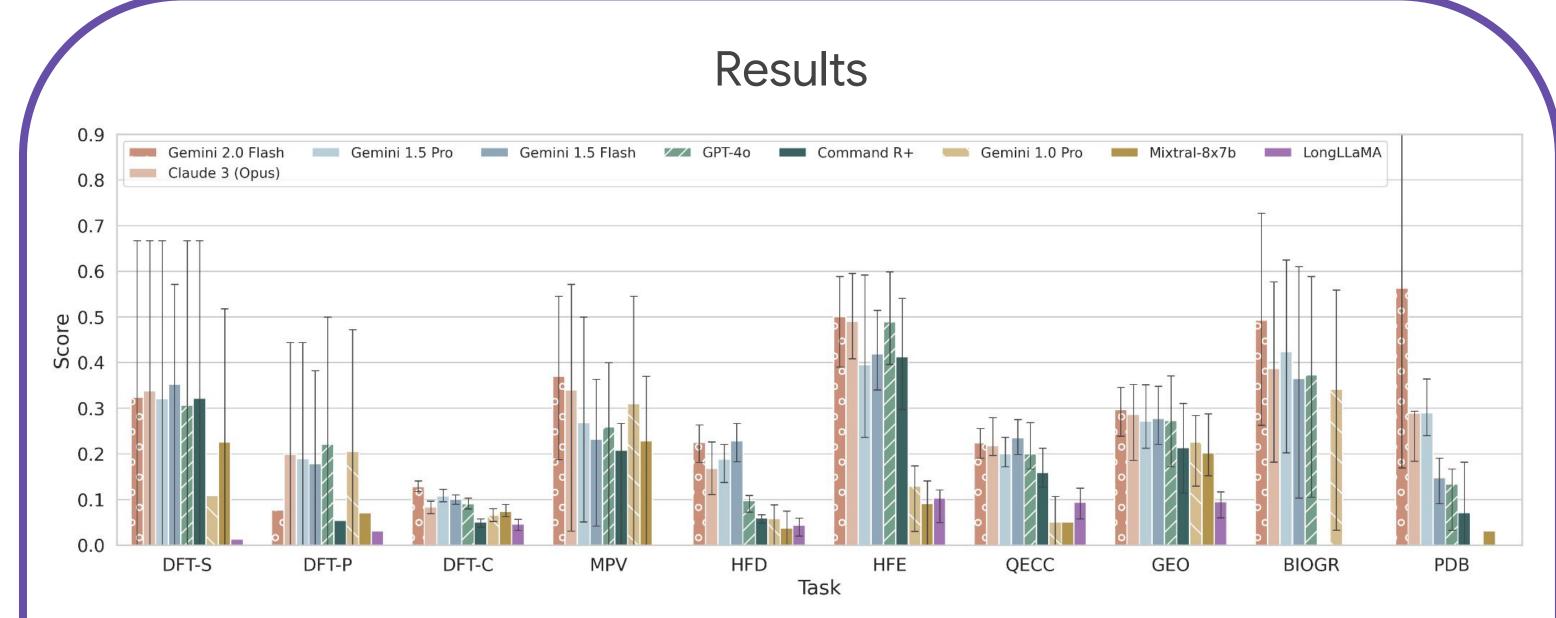


Primary

Output

We collaborated closely with domain experts throughout benchmark development. This included:

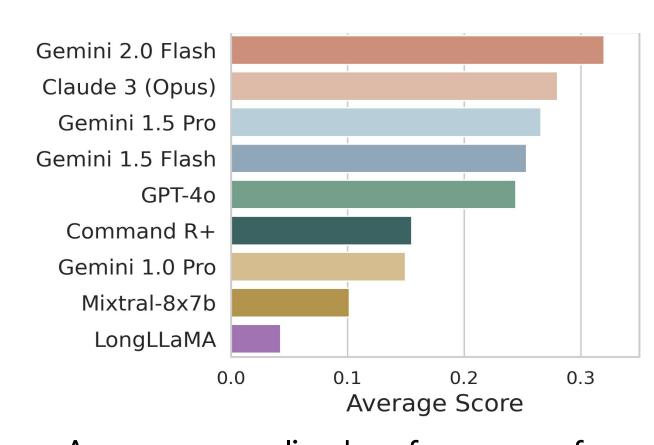
- Defining and identifying tasks reflecting realistic scientific workflows.
- Sourcing relevant papers from the domain.
- Creating accurate, nuanced, and comprehensive ground truth answers.
- Rating task difficulty based on salient features.
- Identifying and verifying evaluation metrics against expert judgments of model responses.



Per task normalized scores of various LLMs on the CURIE benchmark to measure performance on 10 long-context tasks requiring expertise across six scientific disciplines. Higher is better.

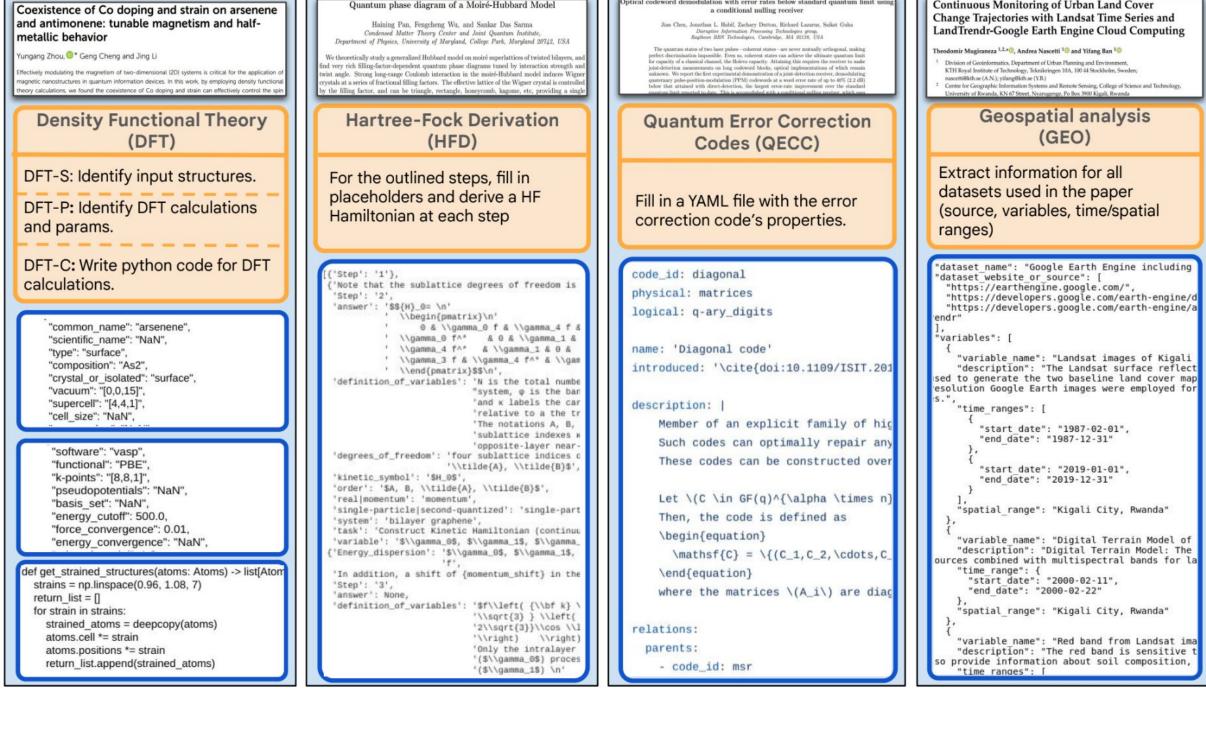


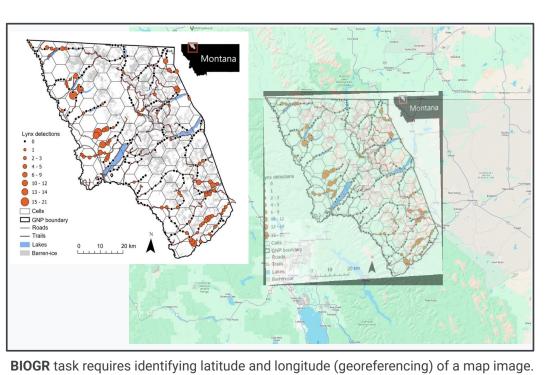
- Gemini Flash 2 and Claude-3 do better. They understand the purpose of the extraction tasks and group responses.
- Exhaustive retrieval e.g. DFT-S, MPV, GEO are challenging for all.
- Flash 2 generated code to solve PDB ~50% of the time and was correct. When enumerating sequence it was similar to other models.
- Experts noted that summaries generated by models were succinct while including a multitude of details hard to comb out e.g. in QECC, and easy to remove afterwards.

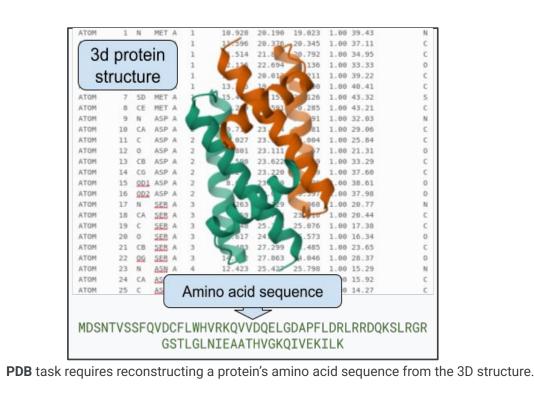


Average normalized performance of long-context LLMs across the 10 tasks from six scientific domains in CURIE.

Illustrative examples of tasks in CURIE







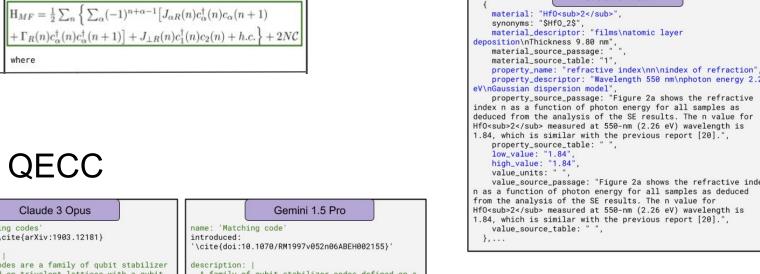
Brief description of tasks and capabilities measured

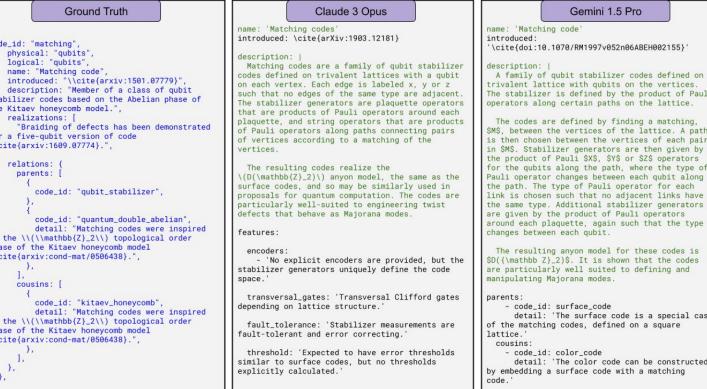
Task	Domain	# Qs	Brief Description	Capability	Format	Eval. Metric
DFT-S	Material Science	74	Extracts input material structures for DFT calculations.	entity recognition, concept tracking	JSON	LLMSim-F1
DFT-P	Material Science	74	Extract parameters for DFT calculations.	concept extraction, tracking, aggregation	JSON	LLMSim-F1
DFT-C	Material Science	74	Write functional code for DFT computations.	concept aggregation, coding	TEXT	ROUGE-L
MPV	Material Science	17	Identify all instances of materials, their properties, and descriptors.	entity recognition, concept extraction, tracking	JSON	LLMSim-F1
HFD	Condensed Matter Physics	64	Derive the Hartree-Fock mean-field Hamiltonian for a quantum many-body system.	concept extraction, algebraic manipulation, reasoning	TEXT	ROUGE-L
HFE	Condensed Matter Physics	19	Extract the most general mean-field Hamiltonian.	concept extraction	TEXT (latex equation)	ROUGE-L
QECC	Quantum Computing	65	Create a YAML file with the Error Correction Code's properties.	concept aggregation, summarization	YAML	ROUGE-L
GEO	Geospecial	15	Extract information for all geospatial datasets used along with the spatial and temporal extents.	concept extraction,	JSON	ROUGE-L
BIOGR	Biodiversity	38	Determine the latitude, longitude bounding box encompassing the region in the map image.	visual comprehension, reasoning	JSON (lat. lon. co-ordinates)	Intersection- over-Union (IoU)
PDB	Protein Sequencing	138	Reconstruct a protein's amino acid sequence form the 3D structure.	tracking, aggregation reasoning	Code or TEXT (seq.)	Identity ratio (IDr)

Tasks in CURIE are varied and have ground truth annotations in mixed and heterogeneous form e.g. as JSONs, latex equations, YAML files, or free-form text. We use programmatic metrics for a predominant number of tasks and propose LLM- based evaluation for others.

Examples

DFT-I	P	DFT-S			
Claude 3 Opus are the details of the DFT calculations in the paper in the specified JSON format: "function_name":"DFT_calculations_1", "software": "GPAW", "functional": "PW91", "k-points": "[2,2,1]", "other_information": "Grid spacing of 0.18 Å. PAW method used to describe effect of er cores on valence electrons. Periodic slab of 4 atomic (110) planes used, with atoms 3 outermost layers allowed to relax. Fixed alloy composition of 6.25% Co (0.25 ML face Co atoms)." "function_name":"DFT_parameters_convergence_tests", "software": "GPAW", "functional: "PW91", "k-points": "Tested (2,2,1), (2,4,1), (2,6,1), (3,4,1), (4,6,1)", "other_information": "Convergence tested with respect to k-points, grid spacing h, smearing of occupation numbers. Binding energies converged within 0.02 eV and surface is free energy within 1 meV/Å*2." "function_name": "DFT_calculations_functional_test", "software": "GPAW", "functional": "Tested PW91, RPBE, vdW-DF2", "*K-points": "NaN", "other_information": "Tested impact of exchange-correlation functional and inclusion van der Waals corrections on binding energies for selected structures. PW91 overbinds bared to RPBE. vdW-corrected binding energies between PW91 and RPBE values." summary, the DFT calculations were performed using the GPAW code with the PW91 hange-correlation functional, a [2,2,1] k-point grid, and a force convergence criteria and the energy cutoff were not provided. HIP LP LP Convergence tests were performed with respect to k-points, grid spacing, smearing, and the impact of the exchange-correlation functional was tested. Key hills like the energy cutoff were not provided.	[[Ground Truth { "common_name": "amphp-aapH", "scientific_name": "h-(4-acetylidene-3-methyl-1-phenyl-2-pyrazolin-5 -one)-4-aminoantipyrine", "type": "isolated molecule", "composition": "NaN", "crystal_or_isolated": "molecule", "scientific_name": "[Mo(NO)2(N-(4-acetylidene-3-methyl-1-phenyl-2-py razolin-5-one)-4-aminoantipyrine)(OH)]", "type": "isolated molecule", "composition": "NaN", "crystal_or_isolated": "molecule", "composition": "NaN", "crystal_or_isolated": "molecule", " " "scientific_name":"N-(4-acetylidene-3-methyl-1-phenyl-2-pyrazolin-5-one)-4-aminoantipyrine", "type": "molecule", "composition": "UNKNOWN", "description": "Pyrazolone Schiff base ligand used to make the Mo complexes", " " " " "id":"structure_metadata_2", "common_name":"[Mo(NO)2(amphp-aap)(OH)]", "scientific_name": "Dinitrosylmolybdenum(0) complex with N-(4-acetylidene-3-methyl-1-phenyl-2-pyrazolin-5-one)-4-aminoantipyrine and hydroxyl ligands", "type": "molecule", "composition":"UNKNOWN", "description":"UNKNOWN", "descript	[Gemini 1.5 Pro { "id": "structure_metadata_1", "common_name": "dha-aapH", "scientific_name": "N-(dehydroacetic acid)-4-aminoantipyrene", "type": "molecule", "composition": "C18H17N304", "description": "Schiff base ligand; derived from dehydroacetic acid and 4-aminoantipyrine", ". , { "id": "structure_metadata_2", "common_name": "amphp-aapH", "scientific_name": "N-(4-acetylidene-3-methyl-1-phenyl-2-pyrazolin-5-one)- 4-aminoantipyrine", "type": "molecule", "composition": "C21H19N502", description": "Schiff base ligand; derived from 4-aayl-3-methyl-1-phenyl-2-pyrazolin-5-one derivative and 4-aminoantipyrine", "" "common_name": "mphpp-aapH", "scientific_name": "N-(3-methyl-1-phenyl-4-propionylidene-2-pyrazolin-5-one e)-4-aminoantipyrine", "type": "molecule", "composition": "C22H21N502", "description": "Schiff base ligand; derived from 4-acyl-3-methyl-1-phenyl-4-propionylidene-2-pyrazolin-5-one derivative and 4-aminoantipyrine", "type": "molecule", "composition": "GNo(N0)2(dha-aap)(OH)]", "scientific_name": "[Mo(N0)2(dha-aap)(OH)]", "scientific_name": "NNKNOWN", "type": "molecule", "composition": "G18H16M0N407", "description": "dinitrosylmolybdenum(0) complex with dha-aapH Schiff base ligand", "common_name": "[Mo(N0)2(amphp-aap)(OH)]", "scientific_name": "NNKNOWN", "type": "molecule", "common_name": "[Mo(N0)2(amphp-aap)(OH)]", "scientific_name": "NNKNOWN", "type": "molecule", "composition": "C2H18M0Nd05", "description": "G2H18M0Nd05", "description": "G1H18M0Nd05", "description": "G1H18M0Nd05", "description": "G1H18M0Nd05", "description": "G2H18M0Nd05", "description": "G2H18M0Nd05", "description": "G2H18M0Nd05", "description": "G2H18M0Nd05", "description": "G2H18M0Nd05", "descripti	[("id": "structure_metadata_1", "common_name": "dha-aapH", "type": "molecule", "composition": "C15H15N303", "description": "Schiff base ligand", " ("id": "structure_metadata_2", "composition": "Schiff base ligand", ("id": "structure_metadata_2", "common_name": "amphp-aapH", "scientific_name": "N-(4-acetylidene-3-methyl-1-phenyl-2-pyrazolin-5-one)-4-aminoantipyrine", "composition": "C2HZ0N402", "description": "Schiff base ligand", ("id": "structure_metadata_3", "common_name": "mphpp-aapH", "scientific_name": "N-(3-methyl-1-phenyl-4-propionylidene-2-pyrazolin-5-one)-4-aminoantipyrine", "scientific_name": "Schiff base ligand", "composition": "C2HZ2N402", "description": "Schiff base ligand", " ("id": "structure_metadata_4", "composition": "Schiff base ligand", "; "scientific_name": "Nitric oxide functionalized molyddenum(0) complex with dha-aapH', "type": "molecule", "composition": "Mo(NO)2(dha-aap)(OH)", "description": "Mo(NO)2(15H14N303)(OH)", "description": "Mo(NO)2(2mphp-aap)(OH)", "composition": "No(NO)2(2mphp-aap)(OH)", "composition": "No(NO)2(2dH19N402)(OH)", "description": "Mo(NO)2(2dH19N402)(OH)", "description": "Mo(NO)2(2dH19N402)(OH)",	
[Ground Truth { "arxiv_id": "2111.09813",	Gemini 1.5 Pro sponse_text": "The general Hartree-Fock Hamiltonian		MPV		





"Hamiltonian": "The general Hartree-Fock

 $H_{MF} = \frac{1}{2} \sum_{n} \left\{ \sum_{\alpha} (-1)^{n+\alpha-1} \left[J_{\alpha R}(n) c_{\alpha}^{\dagger}(n) c_{\alpha}(n+1) \right] \right\}$

 $\Gamma_R(n)c_{\alpha}^{\dagger}(n)c_{\alpha}^{\dagger}(n+1)$ + $J_{\perp R}(n)c_{1}^{\dagger}(n)c_{2}(n) + h.c.$ + 2

Ground Truth rial: "Hf0₂", nyms: "\$Hf0<z\$", rial.descriptor: "films\natomic layer on\nThickness 9.80 mm", rial.source_passage: "", rial.source_table: "", erty_descriptor: "Wavelength 550 mm\nphoton energy 2.26 sas a function of photon energy for all samples as from the analysis of the SE results. The n value for 2</sub> measured at 550-mm (2.26 eV) wavelength is ich is similar with the previous report [20].", erty_source_table: "", value: "1.84", e_units: "", value: "1.84", e_units: "", value: "1.84", e_units: "", value: "1.84", e_source_passage: "Figure 2a shows the refractive index unction of photon energy for all samples as from the analysis of the SE results. The n value for 2</sub> measured at 550-mm (2.26 eV) wavelength is ich is similar with the previous report [20].", erty_source_table: "", value: "1.84", e_units: "", value: "1.84", e_units: "", value_source_passage: "The n value for Hf02 measured at 550-mm (2.26 eV) wavelength is 1.84, which is similar with the previous report [20].", "value_source_passage: "The n value for Hf02 measured at 550-mm (2.26 eV) wavelength is 1.84, which is similar with the previous report [20].", "value_source_passage: "The n value for Hf02 measured at 550-mm (2.26 eV) wavelength is 1.84, which is similar with the previous report [20].", "value_source_table: "", "value_source_table: "", "value_source_table: "", "value_source_table: "", "value_source_table: "", "value_source_table: "", "value_source_table: "" }, "value_source_table:

