Supporting information for

Accelerating materials language processing with large language models

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Tables

Supplementary Table 1. Summary of comparing GPT-enabled text classification models against the SOTA models

Dataset	Approach	Model	Precision	Recall	Accuracy
Battery-related papers	SOTA	BatteryBERT-cased	96.6%	99.5%	97.5%
	Zero-shot learning	GPT-3.5 (‘text-embedding-ada-002’) with Original labels	63.2%	100%	63.2%
		GPT-3.5 (‘text-embedding-ada-002’) with Crude labels	84.5%	97.9%	87.3%
		GPT-3.5 (‘text-embedding-ada-002’) with Designated labels	88.6%	98.3%	91.0%
		GPT-3.5 (‘text-embedding-ada-002’) with Verbose labels	90.8%	98.9%	93.0%
	Few-shot learning	2-way 1-shot learning with GPT-3.5 (‘text-davinci-003’)	95.0%	98.6%	95.7%
		2-way 5-shot learning with GPT-3.5 (‘text-davinci-003’)	95.0%	99.1%	96.1%
		2-way 5-shot learning with GPT-4 (‘gpt-4-0613’)	95.4%	98.9%	96.3%
	Fine-tuning of GPT	GPT-3 (‘davinci’)	95.8%	98.9%	96.6%

Supplementary Table 2. Summary of comparing GPT-enabled NER models against the SOTA models

Dataset	Approach	Model	Category	Precision	Recall	F1-score
Solid-state materials	SOTA	MatBERT-uncased	APL	83.7%	77.8%	80.6%
			CMT	83.3%	88.9%	86.0%
			DSC	90.3%	94.0%	92.1%
			MAT	87.3%	93.5%	90.3%
			PRO	85.5%	81.0%	83.2%
			SMT	79.1%	83.8%	81.4%
			SPL	87.7%	77.1%	82.1%
	Fine-tuning of GPT	GPT-3 (‘davinci’)	APL	96.4%	71.8%	82.3%
			CMT	94.0%	90.3%	92.1%
			DSC	97.3%	93.0%	95.1%
			MAT	97.5%	91.7%	94.6%
			PRO	95.3%	80.2%	87.1%
			SMT	93.9%	84.7%	89.1%
			SPL	99.8%	80.8%	89.3%
Dopant materials	SOTA	MatBERT-uncased	BASEMAT	-	-	72.0%
			DOPANT	-	-	82.0%
			DOPMODQ	-	-	62.0%
	Fine-tuning of GPT	GPT-3 (‘davinci’)	BASEMAT	93.4%	62.0%	74.6%
			DOPANT	95.6%	64.4%	77.0%
			DOPMODQ	92.7%	59.4%	72.4%
AuNPs	SOTA	MatBERT-uncased	DES	70%	52%	56%
			MOR	83%	64%	70%
	Few-shot learning	Random retrieval with GPT-3.5 (‘text-davinci-003’)	DES	63.2%	68.6%	65.8%
			MOR	97.4%	61.7%	75.6%
		Task	DES	65.1%	80.0%	71.8%

		informed random retrieval with GPT-3.5 (‘text-davinci-003’)	MOR	97.9%	68.0%	80.2%
		kNN retrieval with GPT-3.5 (‘text-davinci-003’)	DES	63.6%	99.8%	77.7%
			MOR	97.7%	83.0%	89.8%
		kNN retrieval with GPT-4 (‘gpt-4-0613’)	DES	69.7%	99.6%	82.0%
			MOR	99.8%	87.7%	93.3%

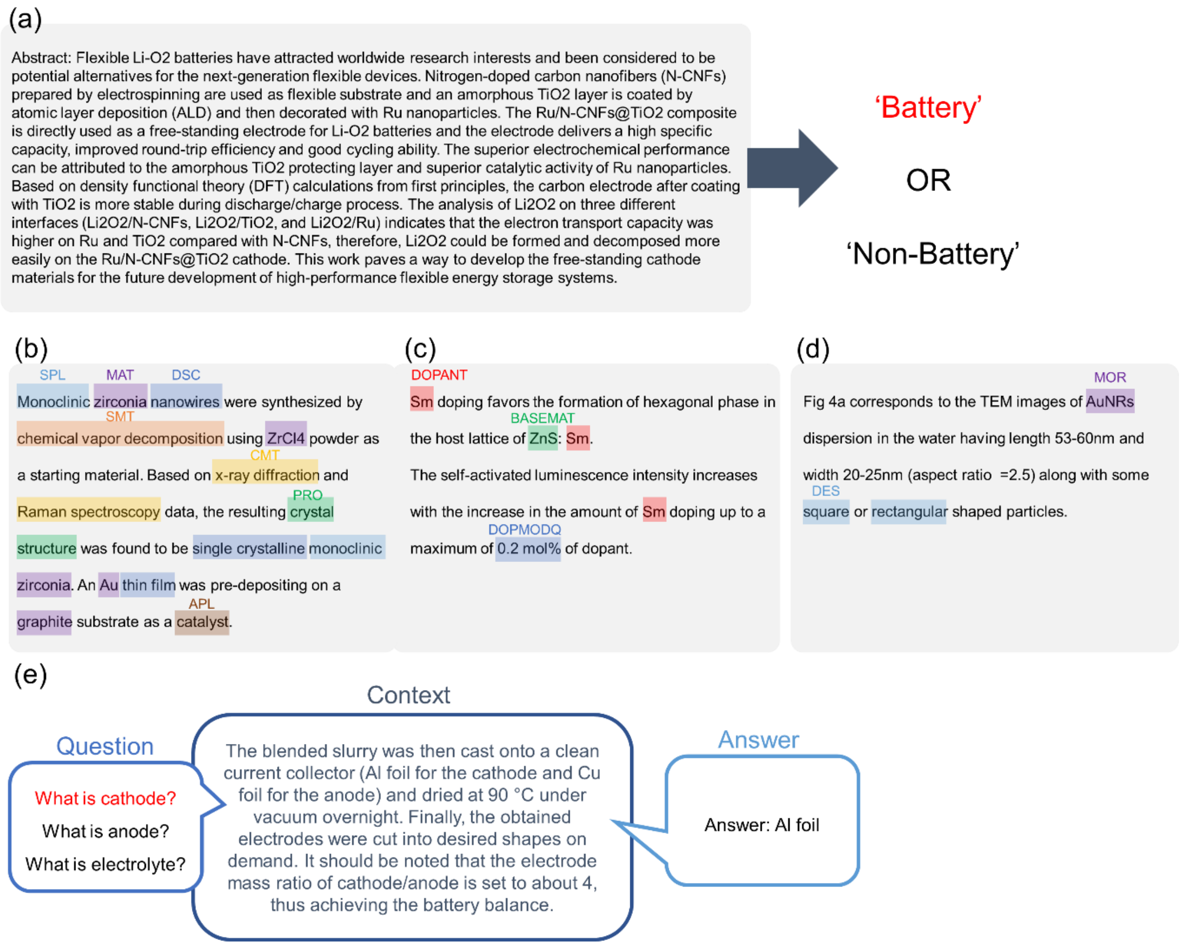
Supplementary Table 3. Summary of comparing GPT-enabled extractive QA models against the SOTA models

Dataset	Approach	Model	Precision	Recall	F1-score
Battery-device QA	SOTA	BatteryBERT-cased	77.49%	71.69%	74.48%
	Zero-shot learning	GPT-3.5 (‘text-davinci-003’)	60.92%	79.96%	69.15%
	Task-informed Zero-shot learning	GPT-3.5 (‘text-davinci-003’)	72.89%	80.65%	76.57%
	Fine-tuning	GPT-3 (‘davinci’)	88.07%	88.35%	88.21%

Label	Publication title	Journal
False	Quality of health care with regard to detection and treatment of mental disorders in patients with coronary heart disease (MenDis-CHD): study protocol	BMC Psychology
	Handwriting capacity in children newly diagnosed with Attention Deficit Hyperactivity Disorder	Research in Developmental Disabilities
	Effects of compensatory cognitive training intervention for breast cancer patients undergoing chemotherapy: a pilot study	Supportive Care in Cancer
	Architecture of fluid intelligence and working memory revealed by lesion mapping	Brain Structure and Function
	Neural correlates of RDoC-specific cognitive processes in a high-functional autistic patient: a statistically validated case report	Journal of Neural Transmission
True	In-operando temperature measurement across the interfaces of a lithium-ion battery cell	Electrochimica Acta
	An all-solid state NASICON sodium battery operating at 200 °C	Journal of Power Sources
	Surface reactions and performance of non-aqueous electrolytes with lithium metal anodes	Journal of Power Sources
	Metal tetrabromophthalocyanines mediate the structure and electrochemical performance of lithium iron phosphate as cathode materials for lithium-ion batteries	Journal of Electroanalytical Chemistry
	Electrochemical characterization of electrolytes for lithium-ion batteries based on lithium difluoromono(oxalato)borate	Journal of Power Sources

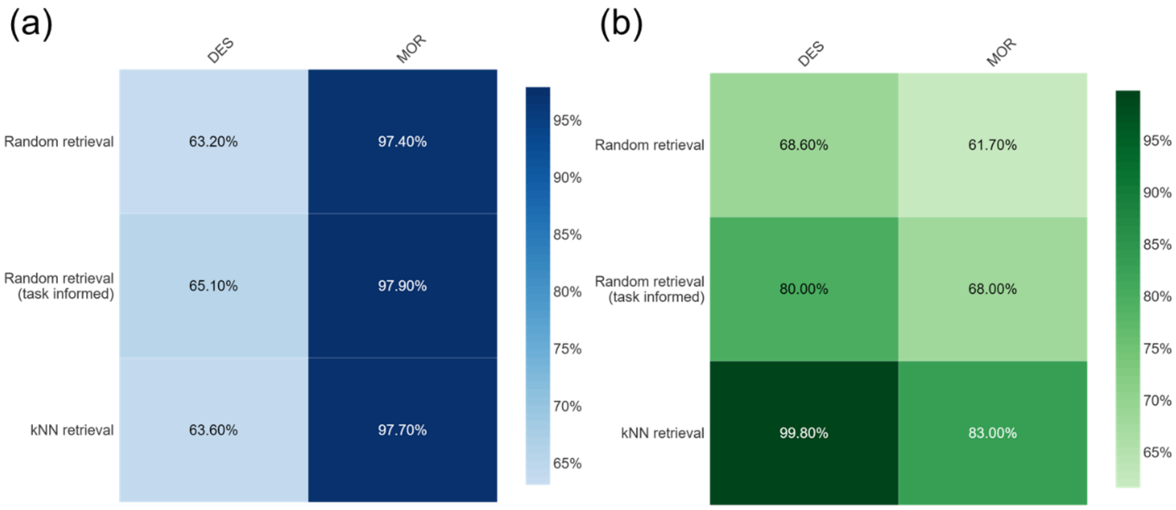
Supplementary Table 4. Parts of text classification dataset for each label. Papers in the False label are related to medical or psychological field applications, while papers in the True label include materials science studies such as battery synthesis, reaction or characterization of materials.

Figures



Supplementary Figure 1. Examples of annotation dataset. (A) Battery-related paper classification dataset (https://huggingface.co/batterydata). This data includes 46,663 labelled papers for which the labels are battery or non-battery are annotated based on their publication sources. The authors defined the battery-related journals and selected the papers in those journals as battery-related papers (ground-truth). **(B)** solid-state materials NER dataset. This dataset includes 800 annotated abstracts. This data set is intended to provide a comprehensive range of relevant information without focusing on any specific aspect of solid materials. Due to the broad definition of entities, solid state data sets usually contain more entities per paragraph. Accordingly, sufficient entity-centric entity tagging prompts could be obtained. **(C)** doped materials NER dataset. This dataset includes 455 annotated abstracts. The process involved annotating tokens on a sentence-by-sentence basis, where each sample corresponds to a single sentence. Sentences were only annotated if they contained precise and direct information about doping in solid-state materials. Accordingly, we tried to apply few-shot learning of GPT 3.5 model rather than prompt-completion fine-tuning module, which requires sufficient number of datasets. **(D)** AuNP synthesis NER dataset. The objective of this dataset is to collect information about the morphologies and descriptions of AuNP from specific sections of full-text literature on AuNP synthesis. A sole annotator annotated a collection of 85 characterization paragraphs extracted from 73 articles related to AuNP synthesis. Similar to doped materials set, we tried to apply few-shot learning of GPT 3.5 model considering the amount of available data. **(E)** battery-device QA dataset. The particular Q&A dataset follows the format of the

SQuAD dataset and includes three types of questions: ‘what is the anode?’, ‘what is the cathode?’, and ‘what is the electrolyte?’.



Supplementary Figure 2. Performance of AuNPs entity recognition of few-shot learning using GPT-3.5 (‘text-davinci-003’) (A–B) AuNPs entity recognition recall and precision of random retrieval, task-informed random retrieval, and kNN retrieval methods. Here, the precision and recall are calculated, after boundary relaxation is conducted on the prediction results. As the entity-wise performances of prior models are not disclosed, we reported the performance of our methods only. In case of DES, random retrieval, task-informed random retrieval and kNN retrieval showed recall values of 63.2%, 65.1% and 63.6%, while precision values are 68.6%, 80.0% and 99.8%. By providing similar examples in the prompt, we were able to obtain high entity recognition performance. In case of MOR, three methods provided high recall of 97.4%, 97.9% and 97.7%, while the precision values are relatively low, 61.7%, 68.0% and 83.0%. Here, we can observe that the effect of adding task-informing sentences is positive on performance, while kNN retrieval strategy is effective in increasing precision performance. This indicates that providing similar examples can help the identification of MOR entities more precisely.

Task: the task is to extract the descriptive entities in the given documents. below are some examples.

prompt: … From the TEM image of Au@PS core – shell particle (Fig . 6) , it is evident that the size of spherical Au particle is ~115 nm , and the outside PS shell (formed by emulsifier - free polymerization) has a thickness of 2–3 nm …

==>\n **completion:** … From the TEM image of Au@PS core – shell particle (Fig . 6) , it is evident that the size of @@spherical## Au particle is ~115 nm , and the outside PS shell (formed by emulsifier - free polymerization) has a thickness of 2–3 nm … \n\n###\n\n

prompt: … Rhombic dodecahedral gold nanocrystals bounded exclusively by { 110 } surfaces were synthesized following our reported procedure . Edge- and corner - truncated octahedral nanocrystals contain significant { 110 } faces from the truncated edges . …

==>\n **completion:** ... @@Rhombic dodecahedral## gold nanocrystals bounded exclusively by { 110 } surfaces were synthesized following our reported procedure . Edge- and corner - truncated @@octahedral## nanocrystals contain significant { 110 } faces from the truncated edges . ... \n\n###\n\n

prompt: … Strong interactions of rod – rod , and rod – plane here may favor the multiple - ring formation for the gold nanorod suspension , differing from the interactions of sphere – sphere and sphere – plane for the spherical gold nanoparticles . …

==>\n **completion:** … Strong interactions of rod – rod , and rod – plane here may favor the multiple - ring formation for the gold nanorod suspension , differing from the interactions of sphere – sphere and sphere – plane for the @@spherical## gold nanoparticles . … \n\n###\n\n

prompt: ... Fig . 1(c) clearly indicates that the SiO2@Au core – shell NCs synthesized were speckled particles i.e. , they retain the gold particle size as was used in the formation of core – shell particles . ... ==>\n

Result: ... Fig . 1(c) clearly indicates that the SiO2@Au core – shell NCs synthesized were speckled particles i.e. , they retain the gold particle size as was used in the formation of core – shell particles . ... \n\n###\n\n

Supplementary Figure 3. Example of few-shot learning prompt based on kNN similar examples; The prompt consists of task information, 3-shot (prompt-completion pairs), and new input.