Using keywords to perform very specific searches in ICSD

In the context of the ever-increasing demand for energy, batteries play a decisive role as storage devices for excess energy and as "mobile" energy suppliers for applications such as those in the automotive industry. At present, batteries based on lithium ions or lead accumulators are mainly used. But whether these concepts can satisfy the constantly growing demand is questionable. For example, lithium-ion batteries also require other rare elements such as cobalt, so that economic and environmental aspects must also be taken into account. The toxicity of lead has been known for a long time and thus limits possible applications.

In the review article "The Aluminum-Ion Battery: A Sustainable and Seminal Concept?", Leisegang et al. (1) describe the importance of battery solutions alongside the two currently most important lithium-ion and lead batteries. The focus of the work in the review article is on concepts based on aluminum ions, which have great advantages over existing batteries. However, research and development on aluminum-ion batteries is still in its infancy and various problems have to be solved (Table 1).

Advantages	Disadvantages/challenges
Theoretically high energy density	Electrolytes require special properties, therefore difficult to find
Infrastructure available for production and recycling	Oxide layer prevents dissolution of aluminum, therefore the redox potential can become more positive
Cheap	Lower redox potential than Li
Non-toxic	High affinity for oxygen (oxide layer)
Air-insensitive	Research lags about 30 years behind Li research

Table 1: Advantages and disadvantages/challenges of aluminum-based batteries

Leisegang et al. go into detail on individual aspects (anode, cathode, electrolyte) and provide interesting potential new materials for use in aluminum-ion batteries based on different theoretical approaches in combination with a screening of the ICSD database. How well these potential candidates perform needs to be tested in practice.

The inclusion of keywords for new entries in ICSD (2) allows for searches that can be much more specific with regards to certain material properties or applications. Since these keywords are only included since 2016, only the newest entries and hence the newest research trends are covered, but the use of keywords will be steadily expanded. The keywords assigned in ICSD describe material properties, analysis methods used or technical fields of application. This information is usually more specific than what is provided by the authors as keywords and often includes more information than can be deduced from the abstract alone.

With the use of relevant keywords in ICSD one can not only confirm the statements regarding the priority of the research as stated in the review article by Leisegang et al., but also provide further information about potential candidates in general based on the experiments that have been

performed by the original authors. A search in ICSD using keywords for materials with a potential application in the field of batteries provides the results shown in Table 2.

Keywords	All Elements	Li	Al (no Li)
Battery/Batteries	483 (109)	278 (71)	8 (0)
Electrolyte/Electrolytes	73 (0)	10 (0)	10 (0)
Electrode/Electrodes	76 (1)	25 (0)	0 (0)
Conductivity	1153 (32)	120 (0)	26 (1)
Channel	2 (0)	0 (0)	1 (0)

Table 2: Results from searches in ICSD for certain battery-related keywords in combination with an element search for Li (and/or anything else) or Al (without Li). In brackets are given the results for the same searches but only for theoretical structures (2).

An application as electrode material does not seem to have been seriously considered yet. Rather, aluminum has so far mainly been considered as a possible (solid-state) electrolyte in battery research, as these Al-types of compounds often have channels within the crystal structure (Fig. 1).

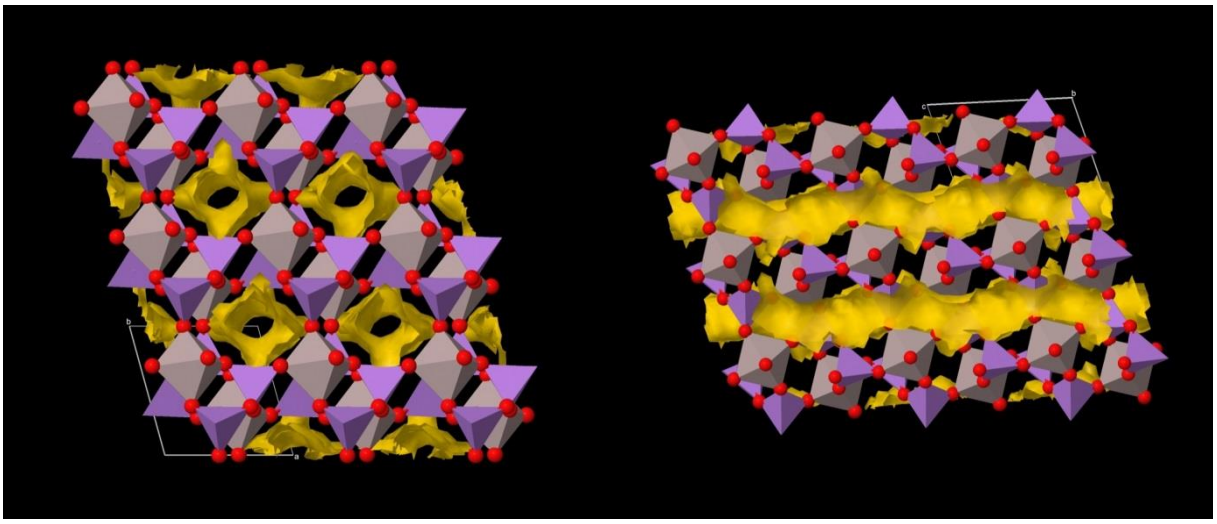

Figure 1: Crystal structure CC 243536 with keyword "channel" (see Table 2). The framework of Al/Cr, As and O forms channels within the crystal structure, which are normally filled with cations (in this structure the cation is potassium, but it was deleted to show the channel). Left: View along the c-axis; Right: View along the b-axis.

Reference:

1) Leisegang, T., Meutzner, F., Zschornak, M., Münchgesang, W., Schmid, R., Nestler, T., Eremin, R. A., Kabanov, A. A., Blatov, V. A. & Meyer, D. C. (2019). The Aluminum-Ion Battery: A Sustainable and Seminal Concept? *Front. Chem.* 7:268, 10.3389/fchem.2019.00268.
2) Zagorac, D., Muller, H., Ruehl, S., Zagorac, J. & Rehme, S. (2019). *J. Appl. Cryst.* 52, 10.1107/S160057671900997X, in press.