Tracking materials science data lineage to manage millions of materials, experiments, and analyses

Edwin Soedarmadji [a], Helge S. Stein [a], Santosh K. Suram [b], Dan Guevarra [a], John Gregoire [a]*

Supplementary Information

Guidelines for conducting searches on the web interface

After the search keyword is submitted, there are three possible scenarios. First, the system returns no result whatsoever. Usually, users can already anticipate this from the empty dropdown feedback. This may mean the search keyword was too narrow, misspelled, or not found in the index. In the second scenario, the search keyword is not specific enough, resulting in far too many items. In this scenario, a subset of the results is returned along with a warning message to the user, alerting to the need to modify the search keywords. Finally, in the third scenario, the search returned results without any warning. In the last two scenarios, users can restrict the result set further by applying filters or by submitting another search keyword. If a new filter is applied to a result set, the system allows users to retrieve the previous sets and if needed, return to the filtered sets if needed.

The set of available filters are dynamic. They are dependent on the result set returned from a search keyword and their associated attributes. These attributes are first grouped by categories containing distinct values with their respective tallies. The categories, the values within the categories, and the value tallies were displayed to the users and available as filtering options with checkboxes. By default, filter categories are combined using the AND operator and category values are combined using the OR operator. However, users can override this default setting. On each filter category, a checkbox for changing the OR operator to AND is provided. Clicking any of these AND checkboxes will revise the result set and an updated filter set tallies. Users can still return to the previous results by clicking on the left arrow and the later results by clicking on the right arrow.

The middle section of the web application shows all the items matching the search keyword plus the entire set of applied filters. The resulting items are plates, runs, experiments, analyses that are identified by their serial numbers for plates and the date they were created for the other item types. The main attributes for plates such as substrate, sample map used for printing, and elements deposited on the plates are all displayed on each box representing the plate. To help with identifying these items, they

are color coded with element symbols, item types, and experiment types (for example electrochemical, uv-vis, etc.)

For runs, the plates under measurement, description, and other important experiment attributes provided by the researchers are included. For experiments and analyses, experiment type and the associated runs are listed for reference. All runs, experiments, and analyses are tagged with the color-coded element symbols. The items displayed in the middle portion of the web application adjust automatically to the filters set on the left portion. Whenever a new checkbox is selected or an existing one deselected, items are added or removed from the list. The application also changes this list as users go up and down the filter history.

When an item box is clicked, the user can view a large portion of the metadata accompanying the item on the right hand section of the web application. This metadata lists the files included, such as raw spectra, electrical signal measurement, or other files produced by the instruments. Clicking any of these item in the list will open a panel that displays the content of the file. By clicking several of these files, users can compare the measurement values obtained from different samples.

The detailed pane also features a button that allows users to display the figures of merit contained in the data item in either the composition space, or on the plate space. Various color schemes and other display options are available to let users quickly isolate samples and files of interest.

Finding previously-published data in MEAD

Table S1: A list of plates used in previous publications. The .info files for these plates contain the .rcp, .exp and .ana files, a subset of which are the basis for the respective publication.

publication doi	plate_id in MEAD
10.1021/co5001579	557
10.1002/celc.201300229	632
10.1038/s41597-019-0019-4	1014,1097,1098,1100,1105,1112,1186,1187,1191,1196,1200,1206, 1231,1234,1304,1328,1469,1477,1517,1520,1527,1529,1530,1533, 1536,1839,1845,1865,1881,1895,1900,1929,1933,1952,1969,2045, 2054,2056,2125,2176,2184,2194,2197,2206,2210,2211,2217,2227, 2324,2334,2336,2360,2363,2370,2371,2380,2608,2612,2660,2661, 2671,2679,2685,2690,2733,2815,2818,2821,2822,2824,2827,2828, 2832,2834,2836,2872,2879,2888,2894,2903,2904,2907,2921,2932, 2935,2999,3005,3009,3028,3123,3124,3151,3326,3400,3402,3407, 3424,3793,3882,3883,3893,3906
10.1557/jmr.2014.296	1015,975,977
10.1002/aenm.201500968	1381,1401,1400,1260
10.1073/pnas.1619940114	1401,1381,3448,3202,3221,3227,3205,3434,3218,3214
10.1021/acscombsci.7b00143	1563,2029
10.1021/co500148p	1696,1693,1712,1698,1697,1472,1627,1709,1713
10.1007/s12678-014-0237-7	1712,1710,1706
10.1063/1.4905365	1959
10.1021/acscombsci.6b00053	2132,3262,1381

10.1021/acsami.6b06714	2152,2345,2154,2994
10.1039/C6TA04746G	2153,2155,3259,1264
10.1039/C5EE03488D	2154,2992
10.1021/acsaem.8b01377	2155,3259
10.1039/C6TA01252C	2197,2227,2200,2194,2137,2123,2224,2226
10.1002/aenm.201401840	2197
10.1021/acs.chemmater.7b03591	2334,3209
10.1021/acscombsci.6b00153	2429
10.1039/C6CP00473C	2643,2430,2640,1400,1401
10.1039/c7cc08002f	2851,2797
10.1021/acsenergylett.7b00607	3050,3216,2655,3051,2848,2656,3059,2851,3068,3199,3046,3066
10.1021/acscombsci.6b00054	3262
10.1021/acs.chemmater.7b03980	3434
10.1039/C8MH01641K	3487,3491,3496,3499,3500,3841,3844,3850,3851,3860,3861,3862, 3863,3868,3869,3871
10.1021/acsenergylett.8b01514	3573,3565,4001,3105,2782
10.1021/acscatal.8b02689	4147,4409,3216,3072,3279
10.1039/C3EE43683G	557,549,483
10.1002/celc.201300229	622,632
10.1021/acscatal.6b03126	632
10.1002/celc.201402149	865