AFLUX: The LUX materials search API for the AFLOW data repositories

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Automated computational materials science frameworks rapidly generate large quantities of materials data useful for accelerated materials design. We have extended the data oriented AFLOW-repository API (Application-Program-Interface, as described in Comput. Mater. Sci. 93, 178 (2014)) to enable programmatic access to search queries. A URI-based search API (Uniform Resource Identifier) is proposed for the construction of complex queries with the intent of allowing the remote creation and retrieval of customized data sets. It is expected that the new language AFLUX, acronym for Automatic Flow of LUX (light), will facilitate the creation of remote search operations on the AFLOW.org set of computational materials science data repositories.

I. INTRODUCTION

Automated computational materials science frameworks such as AFLOW [1–7] rapidly generate large quantities of materials data, which can be used to identify trends, build machine learning models [8–11] and finally accelerate materials design [12]. The dissemination of such large quantities of data requires the use of online advanced databases such as AFLOW.org [13–15], NoMaD [16], Materials Project [17], OQMD [18] and AllIDA [19, 20] to make the data accessible in an effective fashion.

The AFLOW data repositories [13–15] currently contains in excess of 1.5 million materials entries, and over 150 million materials properties (keywords) which are directly accessible using the existing AFLOW data REST-API [15]. The existing data API presents data effectively, but it does not enable programmatic access to the types of complex search queries available through the AFLOW online web portal. In order to address these issues, we have implemented a URI-based search API (Uniform Resource Identifier) which enables the construction of complex search queries and allows for the creation and retrieval of customized data sets.

For large, automatically generated datasets such as those contained in the AFLOW repository, automated verification procedures for calculation quality becomes an important issue, as it is impossible for a user to individually check the calculations for every single entry in a data set. The AFLUX search API can be used to help facilitate such verification checks, since it is possible to include properties which provide information about calculation quality in the results returned by a search query, or even to filter the results to remove entries which do not fulfill specified convergence criteria. To facilitate this, the AFLOW data REST-API has been extended to include additional keywords to expose information concerning the calculation settings and convergence. This upgraded version of the data API is termed version 1.2 as compared to version 1.0 described in Ref. 15. Even and odd version numbers correspond to stable and developmental iterations, respectively.

II. AFLUX SEARCH API

Access to relational information is typically a highly involved process that requires specialized knowledge not generally available or readily attainable by general consumers of said information. An access mechanism that exposes the data to human directed exploration via a graphical user interface (GUI) is typically limited by the GUI designers imagined end use of the data, and is practically impossible to access via programmatic methods. Exposing data via a procedural approach, such as using Structured Query Language (SQL), requires specialized knowledge of both the language in use and the (often highly convoluted) organization of the underlying data. In order to address these concerns we created a domain agnostic text based search application programming interface (API) named LUX. We present LUX in the AFLOW domain context as AFLUX with the design goals of exposing an API that is human accessible, logically robust, concise and as lucid as possible.

A. Design Specification

The design of this API is driven by the need for a straightforward and globally accessible representation of the AFLOW search features. The feature set should reflect and extend the capabilities found in the AFLOW online search GUI available at aflow.org. Further motivation
comes from the attempt to unburden the end user from needing to understand the intricacies of SQL or a particular database schema. An additional benefit of eliminating the explicit representation of the database (DB) schema is that we are free to optimize the internal DB structure without breaking backwards compatibility in the AFLUX API. Although LUX is designed to operate in an origin agnostic fashion, we must make concessions to older software stacks that may be unable to create an extended length URI, and thus LUX strives to balance conciseness with human readability. As a final consideration, the LUX syntax should be generally extensible, both to accommodate the growth of the underlying data and to allow LUX’s application to an arbitrary data store. The LUX syntax was conceived out of these requirements, and for the purpose of this presentation LUX will be described in the AFLUX context. The LUX API language construct is superficially like a C/C++ style subroutine / function call, which we call a matchbook. The utility of LUX is derived from the fact that the intra-matchbook restrictions and inter-matchbook declarations are logically related search criteria.

B. URI Query Context

The implementation of the LUX search API will use an internet URI as the submission layer. In a related effort, the AFLLOW data API also uses a URI to access large data stores [15]. However, in the data API the path portion of the URI is used to uniquely identify each material and navigate between materials, while the query portion of the URI is used to isolate specific data values and dictate the associated data response format. In using the LUX API to summons data the query portion of a URI is more suited to the highly dynamic nature of LUX’s relational criteria.

The beginning of the query section in the URI is defined by the presence of the first question mark character “?” in the URI. The query section is terminated by either the presence of the fragment section, indicated by the first octothorpe character “#”, or by the end of the URI.

Thus the standards for the query portion of a URI forms the foundation of the LUX API.

C. Summons Syntax

The summons syntax is broken into two segments with URI query safe characters forming the body of the summons, as shown in Fig. 1(a). The first portion contains the relational property match criterion with its respective matching restrictions - this is the Matchbook. The Matchbook portion is followed by the Directive portion with its attendant attributes. While there is no a priori order dependency within the Matchbook or the Directives, the Matchbook must come entirely before the Directives in the submitted URI, as shown in Fig. 1.

The property matchbook portion is mandatory for a meaningful data response. In contrast a directive only summons may return metadata or an error state, depending on the directive of concern and the manner in which is is summoned.

D. Character Set

As one of the primary design objectives of LUX is to be human readable, we must consider the allowed URI characters in that context. The URI generic syntax (RFC3986 [21]) defines the explicit restrictions on URI query formation in ABNF notation [22]. As we want our search syntax to be human readable, we will limit our overt use of percent (pet) encoded characters. Finally, in order to support a concise summons we have opted to forgo verbose operators and use single character operators. What follows is a derivation of the LUX character set based on our design goals and the limitations of the standards that LUX will operate under.

From section 3.4 of Ref. 21 the query section of the URI allows for the use of the following characters

\[
\text{query} = *( \text{pchar} / \text{"/"} / \text{"?"} )
\]

which can be read as follows: allow zero or more of the characters from the conjunction of the pchar set, the solidus character “/”, and the question mark character “?”, where the “pchar” character set is defined in section 3.4 of Ref. 21 as

\[
\text{pchar} = \text{unreserved} / \text{pct-encoded} / \text{subdelims} / \text{"/"} / \text{"@"}
\]

“Unreserved” is defined in section 2.3 of Ref. 21 as

\[
\text{unreserved} = \text{ALPHA} / \text{DIGIT} / \text{"-"} / \text{"."} / \text{"/"} / \text{"@"}
\]

and “sub-delims” are defined in Section 2.2 of Ref. 21 as

\[
\text{sub-delims} = \text{"!"} / \text{"$"} / \text{"&"} / \text{"'"} / \text{"("} / \text{"\""} / \text{"\^"} / \text{"\_"} / \text{"\{""} / \text{"\}"} / \text{"\|"} / \text{"\~"}
\]

So, in summary, a strict superset of the characters that our syntax may be constructed from is as follows:

\[
\text{ALPHA} / \text{DIGIT} / \text{"-"} / \text{"."} / \text{"/"} / \text{"@"} / \text{"\^"} / \text{"\~"}
\]

However, while this is the latest relevant RFC there are older protocols implemented by browsers/servers/languages that interfere with the query character set. For instance, RFC1630 and RFC2396 reserved the plus sign. We will attempt to avoid any characters that may result in an unintended mangling of the query.
FIG. 1. (a) URI format for LUX search query. Note that the entire Matchbook must be before all of the Directives. (b) Example search query for a material to act as an electrically insulating heat sink. (c) Results returned in HTML format.

E. Operator Character Codex

We are not explicitly limited by any origin standards, such as HTML5 which only allows unreserved and pct-encoded, as the origin of the query is application agnostic and only requires the ability to construct a valid URI. As an aside, it is often possible to work around the limitation of origin standards by calling lower level methods in the application stack. In essence we need only open a bidirectional communication socket to the LUX API, send an un-mangled URI with an appropriate query structure to the server, and accept the returned data set. That said, we want to make the implementation as easy, unambiguous and unimpeded as we can. As a first consideration we will avoid the use of “?” , “&”, “+”, “;” and “=” in order to avoid confusing arbitrarily handled webserver/cgi/PHP/Web-Browser/... URI parsers. This will also help distinguish LUX from preconceived end user expectations of other, more simplistic, query based API behaviors. We also reserve “.” and “,” as they are inherent to the definition of a number. Furthermore, we want to use ALPHA/DIGIT as general string/number characters.

Lastly we reserve “_” as we use it in the keyword (AFLOW Snake Case keywords for instance) identifier amalgamation convention. This leaves

_ / * / , / : / @ / / .

Thus we define the LUX operator tokens as shown in Table I.

F. Properties are Reserved Words

In addition to the character limitations as defined by the operator character codex there exist reserved words. These words fall into two categories: domain specific (e.g. AFLOW properties) keywords and LUX directives. The list of the AFLOW property data keywords valid as of this draft are those keywords in the original AFLOW data REST API [15] and recently developed keywords given in Appendix B.
TABLE I. LUX Codex. List of the symbols used to represent logic operations in the LUX Search-API syntax. Note that three symbols are currently reserved for future use.

| Logic operation  | Operator symbol | Description                              |
|------------------|-----------------|------------------------------------------|
| BLOCK-NEW        | (               | The new set precedence context           |
| BLOCK-END        | )               | The end set precedence context           |
| UNARY-MUTE       | $               | The property output suppression operator |
| UNARY-NOT        | !               | The logical inversion unary operator     |
| UNARY-LOOSE      | *               | The positional loose datum match unary operator |
| BINAL-AND        | ,               | The logical conjunction binary operator/list separator |
| BINAL-OR         | :               | The logical disjunction binary operator/list separator |
| DATUM-STR        | '               | The explicit string datum context        |
| RESERVED         | @               | Reserved for future use                  |
| RESERVED         | ~               | Reserved for future use                  |
| RESERVED         | /               | Reserved for future use                  |

TABLE II. Numerical filtering.

| Query syntax | Result description                                      |
|--------------|--------------------------------------------------------|
| <keyword>(1.234) | Return only results where value in <keyword> equals 1.234 |
| <keyword>(11.234) | Return only results where value in <keyword> does not equal 1.234 |
| <keyword>(1.234) | Return only results where value in <keyword> is less than or equal to 1.234 |
| <keyword>(11.234) | Return only results where value in <keyword> is not less than or equal to 1.234, i.e. is greater than 1.234 |
| <keyword>(1.234*) | Return only results where value in <keyword> is greater than or equal to 1.234 |
| <keyword>(!1.234*) | Return only results where value in <keyword> is not greater than or equal to 1.234, i.e. is less than 1.234 |

G. Directives are Pseudo Property Keywords

LUX’s directives do not necessarily have an explicit presence in the output data. Their main purpose is to provide context and affect the way that the output is produced.

The list of directives is intentionally short and is as follows:

[“catalog”, “format”, “help”, “paging”, “schema”].

Directive: catalog

It is often helpful to provide a higher-level abstraction of the data sets available. In AFLOW we need to control which library or libraries of materials we wish to query. The internal implementation of the catalog directive could have been provided as a domain specific keyword if the defining property was guaranteed to be ubiquitous, however this may not be possible for all domains and thus “catalog” has been designated in the directive context to allow for specialized internal handling. Within AFLOW the returned set of material properties can be restricted by the use of the “catalog” directive. The currently available catalogs are: [“icsd”, “lib1”, “lib2”, “lib3”].

By default all catalogs are included in a search request and hence the catalog directive may be overridden in many cases. The principle use scenario for catalog is to restrict the search to a subset of endpoint resources. The catalog directive is called as:

API-Server?<Matchbook>,catalog(library_a)

for just “library_a”; or as

API-Server?<Matchbook>,catalog(library_a:library_b)

to search inclusively in both libraries “a” and “b” (i.e. an entry can be in the conjunction of “a” and “b”).

Directive: format

We need to be able to format output of the resultant data. The currently supported output modifiers are “html” and “json”. Use the “format” keyword to set the output type. The default response is compact JSON, setting “json” explicitly returns a more legible JSON response.

API-Server?<Matchbook>,format(json)
or

API-Server?<Matchbook>,format(html)

Directive: help

The help directive with no arguments will return a response with a summary of the proper syntax and use of LUX. If a specific help context has been internally defined for a keyword, then the keyword may be passed to the help directive to retrieve the associated message, otherwise the response will be the same as if no keyword had been supplied.

API-Server?help()
or

API-Server?help(keyword)

Directive: paging

We need the ability to control the number of responses as some searches may return exceedingly large data sets (potentially exceeding tens of millions of data points). By default we will assume 64 data sets in a response page. This return limit can be overridden with the “paging” directive. In the following examples the n-th page of k data sets can be requested. Paging has special powers; asking for zero results (k = 0) will return the number of matching data sets; asking for the zeroth page (n = 0) will return all matching data sets regardless of k - be careful as this can be a large response! Negating n will change the sort order to descending. The paging directive is called as:

API-Server?<Matchbook>,paging(n)
TABLE III. String filtering.

| Query syntax          | Result description                                      |
|-----------------------|---------------------------------------------------------|
| <keyword>(‘foo’)      | Return only results where the string in <keyword> is exactly “foo” |
| <keyword>(!‘foo’)     | Return only results where the string in <keyword> is not “foo”   |
| <keyword>(‘foo’)      | Return only results where the string in <keyword> ends with “foo” |
| <keyword>(‘foo*)      | Return only results where the string in <keyword> starts with “foo” |
| <keyword>(!‘foo*’)    | Return only results where the string in <keyword> does not start with “foo” |
| <keyword>([^’foo*])   | Return only results where the string in <keyword> contains the substring “foo” |
| <keyword>([^’foo]     | Return only results where the string in <keyword> does not contain the substring “foo” |

TABLE IV. Multiple criteria filtering.

| Query syntax          | Result description                                      |
|-----------------------|---------------------------------------------------------|
| <keyword>(1*,1.234)   | Returns only results where value in <keyword> is between 1.0 and 1.234 |
| <keyword>(1*),<keyword>(1.234) | Logically equivalent to <keyword>(1*,1.234) |
| <keyword_a>(1.234),<keyword_b>(’foo’) | Return results that match for <keyword_a>(1.234) and <keyword_b>(’foo’) |
| <keyword_a>(1.234),<keyword_b>(’foo’) | Return results that match for <keyword_a>(1.234) or <keyword_b>(’foo’) |

or

API-Server?<Matchbook>,paging(n,k)

Directive: schema

The schema directive allows external access to the internal data store metadata. The returned metadata represents useful information about the internal nature of the keyword data allowing an end user to make informed decisions about how to handle the property or properties of interest. The LUX language makes no assumptions regarding the metadata content. This allows freedom in the way that LUX is implemented on the backing store. For the AFLUX instance we expose the AFLUX Data schema to allow many forms of disambiguation in the properties. There are a few metadata values that are of particular interest, specifically (in no particular order) title, type, units and verification. Of particular note is the verification metadata, this exposes a contextually relevant set of certification criteria that lends validity to the property of interest. Each property has a potentially unique set of metadata and should be examined prior to using the property in your research. The following are examples of using the schema directive:

API-Server?schema()  
or  
API-Server?schema(<keyword>)

Nota Bene: Directives are not logical

Directives do not support inter-directive logical relations. Intra-Directive properties are not required to be logically related. Any attempt to depend on a logical relationship involving Directive keywords may not have the desired result. Directive keywords are not interpreted in blocking context. Any attempt to modify precedence by the use of blocking parentheses will likely cause a failure in your request. Directive keywords may return an error state when used as the sole operators in your request.

H. Implicit Procedures

The first match keyword in the matchbook is used as the ordering criteria for the response data set, so that the returned entries are listed in increasing order of the property accessed by that keyword.

In the AFLUX implementation the response always includes the compound formula, the AUID and the AURL; i.e. the keywords compound, auid and aurl are implicitly included in the query [15]. If any of these properties are undesirable then they may be suppressed by application of the suppression operator: e.g. the following will prevent the response from producing the compound property

API-Server?<Matchbook>,$compound.

The first data response is paged with 64 entries per page and retrieval of subsequent pages require an explicit use of the paging directive.

I. Matching Criteria

The AFLUX Search-API can filter for search results that match a range of different criteria, including exact matches and value ranges for both strings and numerical data.

Numerical

For scalar filtering of a single element we have three basic operations and they are

< “equality” | “less” | “more” >

and their inverses, i.e.

< “not equals” | “not less” | “not more” >

The results on a numerical value associated with a particular a keyword can be limited using the syntax shown in Table II. Note that the operations “less than” and “greater than” are constructed by negating the “greater than or equal to” and “less than or equal to” operations, respectively.

Strings

For string matching we use a similar construction, as shown in Table III.
FIG. 2. (a) The AFLUX schema for a particular set of keywords can be retrieved using the “schema” Directive with the appropriate keywords as arguments. (b) The schema includes information on the property type referenced by each keyword, the units that the property is provided in, and a list of other keywords which can be used to validate the convergence and quality of the calculation used to generate that particular property.

Note that the string operator " < " is optional unless the matching string contains a reserved character.

Multiple Criterion

The search described so far only demonstrates a single matching condition, hereinafter referred to as a match. We also support the logical construction of multiple matches, referred to as matchbooks. This is done by the juxtaposition of matches with one of the two list separators, namely " < " the logical or operator and " <, > " the logical and operator. Precedence is maintained by using nested lists. For instance, if we want to match two criteria simultaneously the Matchbook might look as shown in the first row of Table IV. When matching multiple criteria, two forms are possible, as shown in the remaining rows of Table IV.

III. EXAMPLES

A. Search for electrically insulating heat sink material

In this example we introduce the steps to screen for an electrically insulating heat sink material for use in nanoelectronics. We search for a material with a band gap in excess of 6eV which also has a high value of the lattice thermal conductivity. Therefore, as shown in Figure 1(b), the Matchbook is constructed by querying two materials properties keywords. The first keyword is agl_thermal_conductivity_300K, which is the lattice thermal conductivity at 300K as calculated using the AGL quasiharmonic Debye-Grüneisen model as implemented within the AFLOW framework [23–25]. The second keyword is Egap, the electronic structure band gap obtained by taking the difference between the conduction band minimum and the valence band maximum, using the band structure calculated along the high-symmetry paths...
in reciprocal space as defined by the AFLLOW Standard [3, 14]. In this case, we restrict the search to return only materials with a band gap calculated to be greater than 6eV by searching for \(E_{\text{gap}}(6*)\). The Directives come after the Matchbook. In this case there are two Directives, both related to the formatting of the returned output. The \texttt{paging}(-1,20) Directive instructs the API to return the first 20 results in descending order, while the \texttt{format(html)} Directive instructs the API to return the results in HTML format.

The returned results for this search are shown in Figure 1(c). In this case, 911 entries are found in the AFLLOW data repository which match the requested search criteria. The entries are sorted in descending order of the value corresponding to the first property keyword in the matchbook, in this case \texttt{agl\_thermal\_conductivity\_300K}, due to the use of a negative value for the page number in the argument to the “paging” Directive. Therefore, the materials with the highest thermal conductivity which would be most suitable for this application appear at the top of the list, namely two different structural phases of the material BeO.

IV. CONCLUSION

In this article, we have presented AFLUX, a URI-based search API extending the original materials data oriented AFLLOW-API. The syntax of the new materials language AFLUX (LUX for AFLLOW) enables the construction of complex search queries and facilitates the creation of remote operations on the AFLLOW.org repositories. The semantic of AFLUX is transparent and easy to adapt to other materials genome initiatives, such as the Materials Project, NoMaD, OQMD, and AiiDA.

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Appendix A: Syntax Diagrams

In the instantiation of an AFLUX process we accept summons that conform to the following syntax. The LUX syntax is described in ABNF (https://tools.ietf.org/html/rfc5234 and https://tools.ietf.org/html/rfc7406).

\[
\text{Summons} = \begin{cases} 
\text{(Matchbook/Directive)} & \ast \text{(Binal Directive)} \\
\text{Matchbook} = \begin{cases} 
\text{[Unary-Not]} & \text{([Unary-Mute]Datum-string("Match")")/"("Matchbook")"/(Matchbook Binal Matchbook)} \\
\text{Match} = \begin{cases} 
\text{[Unary-Not]} & \text{([Unary-Loose](Datum-string/Datum-number)[Unary-Loose]/"("Match")"/(Match Binal Match)} \\
\text{Directive} = \begin{cases} 
\text{[Unary-Mute]Datum-string("(Datum-string/Datum-number) \ast \text{(Binal (Datum-string/Datum-number))")"}
\end{cases}
\end{cases}
\end{cases}
\end{cases}
\]

Appendix B: Table of Properties and API Keywords

This section includes the new keywords added to the AFLLOW data API since the release of version 1.0 as described in Ref. 15. These include keywords which were added to facilitate verification as well as keywords that were added to provide access to data calculated using the AEL-AGL methodology for thermomechanical properties [23, 24]. The \texttt{kpoints} keyword has also been upgraded from version 1.0 to include the number of kpoints per line segment for the electronic band structure calculation, and the new format is also described below. For each keyword, we list the description, type, inclusion policy and the retrieval syntax.
1. Optional materials keywords (alphabetic order)

- **ael_bulk_modulus_reuss**
  - *Description*. Returns AEL bulk modulus as calculated using the Reuss average.
  - *Type*. number.
  - *Units*. GPa.
  - *Example*. `ael_bulk_modulus_reuss=105.315`
  - *Request syntax*. `$aurl/?ael_bulk_modulus_reuss`

- **ael_bulk_modulus_voigt**
  - *Description*. Returns AEL bulk modulus as calculated using the Voigt average.
  - *Type*. number.
  - *Units*. GPa.
  - *Example*. `ael_bulk_modulus_voigt=105.315`
  - *Request syntax*. `$aurl/?ael_bulk_modulus_voigt`

- **ael_bulk_modulus_vrh**
  - *Description*. Returns AEL bulk modulus as calculated using the Voigt-Reuss-Hill (VRH) average.
  - *Type*. number.
  - *Units*. GPa.
  - *Example*. `ael_bulk_modulus_vrh=105.315`
  - *Request syntax*. `$aurl/?ael_bulk_modulus_vrh`

- **ael_elastic_anisotropy**
  - *Description*. Returns AEL elastic anisotropy.
  - *Type*. number.
  - *Units*. dimensionless.
  - *Example*. `ael_elastic_anisotropy=0.000816153`
  - *Request syntax*. `$aurl/?ael_elastic_anisotropy`

- **ael_poisson_ratio**
  - *Description*. Returns AEL Poisson ratio.
  - *Type*. number.
  - *Units*. dimensionless.
- Example. ael_poisson_ratio=0.21599
  - Request syntax. $aurl/?ael_poisson_ratio

• ael_shear_modulus_reuss
  - Description. Returns AEL shear modulus as calculated using the Reuss average.
  - Type. number.
  - Units. GPa.
  - Example. ael_shear_modulus_reuss=73.7868
  - Request syntax. $aurl/?ael_shear_modulus_reuss

• ael_shear_modulus_voigt
  - Description. Returns AEL shear modulus as calculated using the Voigt average.
  - Type. number.
  - Units. GPa.
  - Example. ael_shear_modulus_voigt=73.7989
  - Request syntax. $aurl/?ael_shear_modulus_voigt

• ael_shear_modulus_vrh
  - Description. Returns AEL shear modulus as calculated using the Voigt-Reuss-Hill (VRH) average.
  - Type. number.
  - Units. GPa.
  - Example. ael_shear_modulus_vrh=73.7929
  - Request syntax. $aurl/?ael_shear_modulus_vrh

• ael_speed_of_sound_average
  - Description. Returns AEL average speed of sound calculated from the transverse and longitudinal speeds of sound.
  - Type. number.
  - Units. m/s.
  - Example. ael_speed_of_sound_average=500.0
  - Request syntax. $aurl/?ael_speed_of_sound_average

• ael_speed_of_sound_longitudinal
  - Description. Returns AEL speed of sound in the longitudinal direction.
  - Type. number.
  - Units. m/s.
  - Example. ael_speed_of_sound_longitudinal=500.0
  - Request syntax. $aurl/?ael_speed_of_sound_longitudinal

• ael_speed_of_sound_transverse
  - Description. Returns AEL speed of sound in the transverse direction.
  - Type. number.
  - Units. m/s.
  - Example. ael_speed_of_sound_transverse=500.0
  - Request syntax. $aurl/?ael_speed_of_sound_transverse

• agl_acoustic_debye
  - Description. Returns AGL acoustic Debye temperature.
- **Type.** number.
- **Units.** K.
- **Example.** agl_acoustic_debye=492
- **Request syntax.** $aurl/?agl_acoustic_debye

- **agl_bulk_modulus_isothermal_300K**
  - **Description.** Returns AGL isothermal bulk modulus at 300K and zero pressure.
  - **Type.** number.
  - **Units.** GPa.
  - **Example.** agl_bulk_modulus_isothermal_300K=96.6
  - **Request syntax.** $aurl/?agl_bulk_modulus_isothermal_300K

- **agl_bulk_modulus_static_300K**
  - **Description.** Returns AGL static bulk modulus at 300K and zero pressure.
  - **Type.** number.
  - **Units.** GPa.
  - **Example.** agl_bulk_modulus_static_300K=99.59
  - **Request syntax.** $aurl/?agl_bulk_modulus_static_300K

- **agl_debye**
  - **Description.** Returns AGL Debye temperature.
  - **Type.** number.
  - **Units.** K.
  - **Example.** agl_debye=620
  - **Request syntax.** $aurl/?agl_debye

- **agl_gruneisen**
  - **Description.** Returns AGL Grüneisen parameter.
  - **Type.** number.
  - **Units.** dimensionless.
  - **Example.** agl_gruneisen=2.06
  - **Request syntax.** $aurl/?agl_gruneisen

- **agl_heat_capacity_Cv_300K**
  - **Description.** Returns AGL heat capacity at constant volume (C_V) at 300K and zero pressure.
  - **Type.** number.
  - **Units.** k_B/cell.
  - **Example.** agl_heat_capacity_Cv_300K=4.901
  - **Request syntax.** $aurl/?agl_heat_capacity_Cv_300K

- **agl_heat_capacity_Cp_300K**
  - **Description.** Returns AGL heat capacity at constant pressure (C_p) at 300K and zero pressure.
  - **Type.** number.
  - **Units.** k_B/cell.
  - **Example.** agl_heat_capacity_Cp_300K=5.502
  - **Request syntax.** $aurl/?agl_heat_capacity_Cp_300K

- **agl_poisson_ratio_source**
– **Description.** Returns source of Poisson ratio used to calculate Debye temperature in AGL. Possible sources include **ael**, in which case the Poisson ratio was calculated from first principles using AEL; **empirical**, in which case the value was taken from the literature; and **Cauchy_ratio_0.25**, in which case the default value of 0.25 of the Poisson ratio of a Cauchy solid was used.

– **Type.** string.
– **Example.** `agl_poisson_ratio_source=ael`
– **Request syntax.** `$aurl/?agl_poisson_ratio_source`

• **agl_thermal_conductivity_300K**
  – **Description.** Returns AGL thermal conductivity at 300K.
  – **Type.** number.
  – **Units.** W/m*K.
  – **Example.** `agl_thermal_conductivity_300K=24.41`
  – **Request syntax.** `$aurl/?agl_thermal_conductivity_300K`

• **agl_thermal_expansion_300K**
  – **Description.** Returns AGL thermal expansion at 300K and zero pressure.
  – **Type.** number.
  – **Units.** 1/K.
  – **Example.** `agl_thermal_expansion_300K=4.997e-05`
  – **Request syntax.** `$aurl/?agl_thermal_expansion_300K`

• **delta_electronic_energy_final**
  – **Description.** Convergence energy threshold for the electronic SCF loop.
  – **Type.** number.
  – **Example.** `delta_electronic_energy_final=0.000071416`
  – **Request syntax.** `$aurl/?delta_electronic_energy_final`

• **delta_electronic_energy_threshold**
  – **Description.** Convergence energy threshold for the electronic SCF loop.
  – **Type.** number.
  – **Example.** `delta_electronic_energy_threshold=0.0001`
  – **Request syntax.** `$aurl/?delta_electronic_energy_threshold`

• **kpoints**
  – **Description.** Set of \text{k}-point meshes uniquely identifying the various steps of the calculations, e.g. relaxation, static and electronic band structure (specifying the \text{k}-space symmetry points of the structure and the number of points per path segment).
  – **Type.** Set of numbers and strings separated by “,” and “;”.
  – **Example.** `kpoints=10,10,10;16,16,16;\Gamma-X,X-W,W-K,K-\Gamma;\Gamma-L,L-U,U-W,W-L,L-K,U-X;20`
  – **Request syntax.** `$aurl/?kpoints`

• **nkpoints**
  – **Description.** Number of \text{k}-points used for the calculation.
  – **Type.** number.
  – **Example.** `nkpoints=2197`
  – **Request syntax.** `$aurl/?nkpoints`

• **nkpoints_irreducible**
- **Description.** Number of k-points in the irreducible Brillouin zone.
- **Type.** number.
- **Example.** nkpoints=2197
- **Request syntax.** $aurl/?nkpoints

* pressure_residual
- **Description.** Returns the residual pressure for the simulation, i.e. the difference between the pressure specified in the input and the actual pressure achieved for the relaxation.
- **Type.** number.
- **Units.** Natural units of the $code, e.g., kbar or a.u. (Ry/Bohr) if the calculations were performed with VASP [26] or QE [27], respectively.
- **Example.** pressure_residual=10.0
- **Request syntax.** $aurl/?pressure_residual

* Pulay_stress
- **Description.** Returns the Pulay stress for the simulation.
- **Type.** number.
- **Units.** Natural units of the $code, e.g., kbar or a.u. (Ry/Bohr) if the calculations were performed with VASP [26] or QE [27], respectively.
- **Example.** Pulay_stress=10.0
- **Request syntax.** $aurl/?Pulay_stress

* stress_tensor
- **Description.** Returns the stress tensor obtained for the simulation.
- **Type.** List of 9 numbers separated by commas, giving the elements of the stress tensor in the form $S_{xx}, S_{xy}, S_{xz}, S_{yx}, S_{yy}, S_{yz}, S_{zx}, S_{zy}, S_{zz}$.
- **Units.** Natural units of the $code, e.g., kbar or a.u. (Ry/Bohr) if the calculations were performed with VASP [26] or QE [27], respectively.
- **Example.** stress_tensor=0.74,0,0,0,0.74,-0,0,-0,-4.42
- **Request syntax.** $aurl/?stress_tensor

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