AFLOW-ML: A RESTful API for machine-learning predictions of materials properties

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Machine learning approaches, enabled by the emergence of comprehensive databases of materials properties, are becoming a fruitful direction for materials analysis. As a result, a plethora of models have been constructed and trained on existing data to predict properties of new systems. These powerful methods allow researchers to target studies only at interesting materials — neglecting the non-synthesizable systems and those without the desired properties — thus reducing the amount of resources spent on expensive computations and/or time-consuming experimental synthesis. However, using these predictive models is not always straightforward. Often, they require a panoply of technical expertise, creating barriers for general users. AFLOW-ML (AFLOW Machine Learning) overcomes the problem by streamlining the use of the machine learning methods developed within the AFLOW consortium. The framework provides an open RESTful API to directly access the continuously updated algorithms, which can be transparently integrated into any workflow to retrieve predictions of electronic, thermal and mechanical properties. These types of interconnected cloud-based applications are envisioned to be capable of further accelerating the adoption of machine learning methods into materials development.

I. INTRODUCTION

Since their inception, high throughput materials science frameworks such as AFLOW [1–8] have been amassing large databases of materials properties. For instance, the AFLOW database [9–12] alone contains over 1.7 million material compounds with over 170 million calculated properties, generated from the Inorganic Crystal Structure Database (ICSD) [13–15], as well as by decorating crystal structure prototypes [16]. Combined with other online databases such as the Materials Project [17], NoMaD [18] and OQMD [19], materials data is abundant and available. As a result, machine learning (ML) methods have emerged as the ideal tool for data analysis [20–25], by identifying the key features in a data set [26] to construct a model for predicting the properties of a material. Recently, several models were developed to predict the properties of various material classes such as perovskites [27, 28], oxides [29], elpasolites [30, 31], thermoelectrics [32–34], and metallic glasses [35]. Additionally, generalized approaches have been devised for inorganic materials [36–43] and for systematically identifying efficient physical models of materials properties [44].

While predictions are powerful tools for rational materials design, the discipline is still reasonably new within the realm of materials science. As a result, a working understanding of machine learning principles, along with a high level of technical expertise, is required for using code bases effectively. This inhibits accessibility, where an average end user aims to utilize the codes to retrieve predictions with as little complication as possible. With the ever increasing number of predictive models, a unique challenge emerges: how does one create an accessible means to integrate machine learning frameworks into a materials discovery workflow?

AFLOW-ML alleviates this issue by providing a simplified abstraction on top of sophisticated predictive models. Predictions are exposed through a web accessible Application Programming Interface (API) where functionality is distilled down to its essence: from the user input, return a prediction. AFLOW-ML can be added into any code base through use of an HTTP request library, native to most languages. Alternatively, AFLOW-ML can be utilized though use of the included Python client and command line interface. Through such abstractions, AFLOW-ML is accessible to a wide audience: it unburdens the user from having to understand the intricacies of machine learning and eliminates the technical expertise required to set up such codes.

II. REST API

The AFLOW-ML API is structured around a REpresentational State Transfer (REST) architecture, which allows resources to be accessed using HTTP request methods. Each resource is located at an endpoint, which is identified by a URL comprised of descriptive nouns.

A URL may also include special variables in the form of path parameters and a query string. A path param-
TABLE I. A list of all endpoints in the API. Actions specify the supported HTTP request method, endpoints define the URL and objects are the returned resource. An endpoint with {...} denotes a path parameter.

| Action | Endpoint | Object               |
|--------|----------|----------------------|
| POST   | /plmf/prediction | task             |
| POST   | /mfd/prediction   | task               |
| GET    | /prediction/result/{id} | status or prediction |

The overall structure of the API can be seen in Table I. All endpoints are located at the base URL aflow.org/API/aflow-ml/v1.0/ and are organized by the model and the returned object.

AFLOW-ML currently supports two models: molar fraction descriptor (mfd) [37] and property-labeled materials fragments (plmf) [36]. It is designed to be extensible, and additional models will be added in the future as they are developed.

The mfd model [37] predicts the material properties based on the chemical formula only: the vector of descriptors has 87 components, each component $b_i$ being the mole fraction of element $Z_i$ in the compound ($Z_1$ is H, $Z_2$ is He, etc.). The model is built with nonlinear support vector machines and a radial basis function kernel. The model is trained using a data set of 292 randomly selected compounds of the ICSD for which the vibrational properties are computed with DFT calculations.

The plmf model [36] represents each crystal structure as a colored graph, where the atomic vertices are decorated by the reference properties of the corresponding elemental species. Topological neighbors are determined using a Voronoi tesselation, and these nodes are connected to form the graph. The final feature vector for the ML model is obtained by partitioning the full graph into smaller subgraphs, termed fragments in analogy with the fragment-based descriptors used in cheminformatics [45]. All plmf models are built with the Gradient Boosting Decision Tree (GBDT) method [46]. Models for electronic and thermomechanical properties were trained on 26,674 and 2,829 materials entries from the AFLOW repository, respectively. All models are validated through $Y$-randomization (label scrambling) and five-fold cross validation.

In general, API usage involves uploading a material structure to a POST endpoint, <model>/prediction, and retrieving a prediction object from a GET endpoint, /prediction/result/{id}, as shown in the flowchart in Figure 1. POST endpoints are responsible for the submission of a material structure for a prediction. In their request body, the file keyword is required. It must contain a string representation of the material’s crystal structure, in POSCAR 5 format (the lattice geometry and atomic position input file for version 5 of the VASP DFT package [47, 48]). Upon receiving a request, the response body returns a task object containing information about the submitted structure, which has the following format:

```json
{
  "id": String,
  "model": String,
  "results_endpoint": String
}
```

When a material is posted to the API, a prediction task is created and added to a queue. Each task is assigned an identifier, the id keyword, used to fetch the the prediction object at the endpoint referenced in the results_endpoint keyword. This endpoint, /prediction/result/{id}, supports the GET method and requires the id as a path parameter. Depending on the status of the prediction task, the response body returns a status object or prediction object. When the task is still in the queue, the status object is returned:

```json
{
  "status": String,
  "description": String
}
```

The status object details the state of the prediction task. The state is identified by the keyword status which takes one of the following values: STARTED, PENDING, SUCCESS and FAILURE, while a description of each status type is given by the description keyword. When attempting to retrieve the prediction object, it is best to poll the endpoint periodically to check the status. Tasks that are still within the queue are given the STARTED or PENDING status, while a completed task status will read SUCCESS. In instances where the uploaded file is incorrectly formatted, a failed task will occur, status: FAILURE. When the task is completed, the response contains the prediction object. The prediction object is an extension of
the status object and contains different keywords depending on the model used. For plmf, the prediction object, known as a plmf prediction, takes the following form:

```
{
    "status": String,
    "description": String,
    "model": String,
    "citation": String,
    "ml_egap_type": String,
    "ml_egap": Number,
    "ml_energy_per_atom": Number,
    "ml_ael_bulk_modulus_vrh": Number,
    "ml_ael_shear_modulus_vrh": Number,
    "ml_agl_debye": Number,
    "ml_agl_heat_capacity_Cp_300K": Number,
    "ml_agl_heat_capacity_Cv_300K": Number,
    "ml_agl_heat_capacity_Cp_300K_per_atom": Number,
    "ml_agl_heat_capacity_Cv_300K_per_atom": Number,
    "ml_agl_thermal_conductivity_300K": Number,
    "ml_agl_thermal_expansion_300K": Number
}
```

The mfd model returns an mfd prediction object:

```
{
    "status": String,
    "description": String,
    "model": String,
    "citation": String,
    "ml_Cv": Number,
    "ml_Fvib": Number,
    "ml_Svib": Number
}
```

The details of each object and their keywords are found in the List of API Endpoints and Objects section.

### IV. USING THE API

The process to retrieve a prediction is as follows: First, the contents of a POSCAR 5 file, titled test.poscar, are uploaded to the submission endpoint. This can be achieved by using an HTTP library such as requests (Python) [49], URLSession (iOS SDK), HttpURLConnection (Android SDK), Fetch (JavaScript) or using a command line tool such as wget or curl. For this example, curl will be used. The contents of the POSCAR are posted to the submission endpoint as follows:

```
curl http://aflow.org/API/aflow-ml/v1.0/plmf/prediction --data-urlencode file@test.poscar
```

where the `--data-urlencode` flag handles encoding the contents of the POSCAR, located in the current directory, and associating it to the file keyword. Note that as mentioned previously, the POST will return a JSON response including the task id. The task id is then used to poll the results endpoint:
curl http://aflow.org/API/aflow-ml/v1.0/prediction/result/{id}

The status keyword is used as an indicator to determine if any additional polling is required. Depending on the status of the job, the endpoint will return either a task status object or a prediction object. If the status keyword’s value is SUCCESS then no additional polling is required, since the endpoint will return a prediction object, which is an extension of the task status object.

V. LIST OF API ENDPOINTS AND OBJECTS

This section includes the details of each endpoint and object accessible in the API. Endpoint information contains the associated HTTP method, request parameters, request body data and response object for each endpoint. Object properties are listed along with their type and description.

A. Endpoints

• POST plmf/prediction
  
  - **Description.** Uploads the contents of a POSCAR 5 to retrieve a prediction using the plmf model.
  
  - **Query parameters.**
    * file (required) - The contents of the POSCAR 5.
  
  - **Response format.** On success, the response header contains the HTTP status code 200 OK and the response body contains a task object, in JSON format.

• POST mfd/prediction
  
  - **Description.** Uploads the contents of a POSCAR 5 to retrieve a prediction using the mfd model.
  
  - **Query parameters.**
    * file (required) - The contents of the POSCAR 5.
  
  - **Response format.** On success, the response header contains the HTTP status code 200 OK and the response body contains a task object, in JSON format.

• GET /prediction/result/{id}
  
  - **Description.** Fetches the status object or returns the prediction object when the task is completed.
  
  - **Path parameters.**
    * id (required) - The unique identifier retrieved from the task object on submission.
  
  - **Query string arguments.**
    * fields - A comma separated list of the fields to include in the JSON response object. Note that specified fields will only affect the prediction object.

  - **Response format.** On success, the response header contains the HTTP status code 200 OK. If the task is still pending, the response body contains a task status object in JSON format. Upon completion the response body contains a prediction object in JSON format.

• Example.

  curl http://aflow.org/API/aflow-ml/v1.0/plmf/prediction
  --data-urlencode file@test.poscar

B. Objects

• Task
  
  - **Description.** Describes the task for a submitted prediction. Includes the unique identifier for the prediction and results endpoint.
  
  - **Keys.**
    * id
      - **Description.** The unique identifier of the prediction task. Used at the fetch prediction endpoint to retrieve the status of a prediction and return the results on completion.
      - **Type.** String.
  
  - **results_endpoint**
    - **Description.** The path of the endpoint where the prediction task status and results are retrieved.
    - **Type.** String.
- **model**
  - **Description.** The name of the machine learning model used to generate the prediction.
  - **Type.** String.

- **Example.**

  ```
  {
  "id": "d29af704-06bf-4dc8-8928-cd2c41aae454",
  "model": "plmf",
  "results_endpoint": "/prediction/result/d29af704-06bf-4dc8-8928-cd2c41aae454"
  }
  ```

- **Status**
  - **Description.** Provides the status of a (prediction) task.

- **Keys.**
  - **status**
    - **Description.** The status of the task. Takes the following values: STARTED, PENDING, SUCCESS and FAILURE. When a task is added to the queue its status will read PENDING. Once it reaches the top of the queue the status will read STARTED and the prediction will run. If the prediction is successful the status will read SUCCESS.
    - **Type.** String.
  - **description**
    - **Description.** Describes the status of the task.
    - **Type.** String.
  - **model**
    - **Description.** The model used in the prediction.
    - **Type.** String.
  - **citation**
    - **Description.** The DOI for the model's publication.
    - **Type.** String.
  - **ml_egap_type**
    - **Description.** Specifies if the material is a metal or an insulator. Takes the following values: Metal, Insulator.
    - **Type.** String.
  - **ml_egap**
    - **Description.** The electronic band gap.
    - **Units.** eV.
    - **Type.** Number.
  - **ml_energy_per_atom**
    - **Description.** The energy per atom.
    - **Units.** eV/atom.
    - **Type.** Number.
  - **ml_ael_bulk_modulus_vrh**
    - **Description.** The bulk modulus, trained using the Automatic Elasticity Library (AEL). [50]
    - **Units.** GPa.
    - **Type.** Number.
  - **ml_ael_shear_modulus_vrh**
    - **Description.** The shear modulus, trained using AEL.
    - **Units.** GPa.
    - **Type.** Number.
  - **ml_agl_debye**
    - **Description.** The Debye temperature, trained using the Automatic GIBBS Library (AGL) [51].
    - **Units.** K.
    - **Type.** Number.
  - **ml_agl_heat_capacity_Cp_300K**

- **plmf prediction**
  - **Description.** The results of the prediction using the plmf model. This is an extension of the task status object.

- **Keys.**
  - **status**
- Description. The heat capacity at 300K and constant pressure, trained using AGL.
  - Units. $k_B$/cell.
  - Type. Number.
* ml_agl_heat_capacity_Cp_300K_per_atom
  - Description. The heat capacity per atom at 300K and constant pressure, trained using AGL.
  - Units. $k_B$/atom.
  - Type. Number.
* ml_agl_heat_capacity_Cv_300K
  - Description. The heat capacity at 300K and constant volume, trained using AGL.
  - Units. $k_B$/cell.
  - Type. Number.
* ml_agl_heat_capacity_Cv_300K_per_atom
  - Description. The heat capacity per atom at 300K and constant volume, trained using AGL.
  - Units. $k_B$/atom.
  - Type. Number.
* ml_agl_thermal_conductivity_300K
  - Description. The lattice thermal conductivity at 300K, trained using AGL.
  - Units. W/(m K).
  - Type. Number.
* ml_agl_thermal_expansion_300K
  - Description. The thermal expansion coefficient at 300K, trained using AGL.
  - Units. K$^{-1}$.
  - Type. Number.

- Example.

```json
{
  "status": "SUCCESS",
  "description": "The job has completed.",
  "model": "plmf",
  "citation": "10.1038/ncomms15679",
  "ml_egap_type": "Insulator",
  "ml_egap": 0.923,
  "ml_energy_per_atom": -5.760,
  "ml_ael_bulk_modulus_vrh": 178.538,
  "ml_ael_shear_modulus_vrh": 140.121,
  "ml_agl_debye": 713.892,
  "ml_agl_heat_capacity_Cp_300K": 23.362,
  "ml_agl_heat_capacity_Cp_300K_per_atom": 2.333,
  "ml_agl_heat_capacity_Cv_300K": 22.625,
  "ml_agl_heat_capacity_Cv_300K_per_atom": 2.311,
  "ml_agl_thermal_conductivity_300K": 2.792,
  "ml_agl_thermal_expansion_300K": 6.093e-05
}
```

- mfd prediction
  - Description. The results of a prediction using the mfd model. This is an extension of the task status object.
  - Keys.
    * status
      - Description. The status of the task. Takes the following values: STARTED, PENDING, SUCCESS and FAILURE. When a task is added to the queue its status will read PENDING. Once it reaches the top of the queue the status will read STARTED and the prediction will run. If the prediction is successful the status will read SUCCESS.
      - Type. String.
    * description
      - Description. Describes the status of the task.
      - Type. String.
    * model
      - Description. The model used in the prediction.
      - Type. String.
    * citation
      - Description. The DOI for the model’s publication.
      - Type. String.
    * ml_Cv
      - Description. The heat capacity at constant volume.
      - Units. meV/(atom K).
      - Type. Number.
    * ml_Fvib
      - Description. The vibrational free energy per atom.
      - Units. meV/atom.
VI. PYTHON CLIENT

A Python client is available for the AFLOW-ML REST API that provides researchers and developers a means to integrate AFLOW-ML into their applications or workflows, such as AFLOWπ [8]. The client includes the AFLOWmlAPI class which provides all the functionality needed to interface with the AFLOW-ML API, and can be downloaded at aflow.org/src/aflow-ml. From the client, a prediction is retrieved by passing the contents of a POSCAR file to the get_prediction method. The AFLOWmlAPI class can be incorporated into a Python framework using code similar to the example illustrated in Figure 2.

```python
from AFLOWml.client import AFLOWmlAPI

with open('test.poscar', 'r') as input_file:
aflowML = AFLOWmlAPI()
data = aflowML.get_prediction(input_file.read(), 'plmf')
```

FIG. 2. Example showing how to retrieve a prediction using the AFLOW-ML Python client.

This method takes two arguments: poscar and model, where poscar is a file object (reading from the file test.poscar in the example in Figure 2) and model is a string specifying the model to use (plmf or mfd). This method returns a Python dictionary, in which the keys and respective predicted values are model dependent. For a list of each prediction object’s key and value pair, please refer to the previous section.

The client’s AFLOWmlAPI class includes two additional methods, submit_job and poll_job, that provide more control when submitting a prediction, and which can be used in place of the get_prediction method in the example shown in Figure 2. The submit_job method targets the <model>/prediction endpoint and returns the jobs task id. From this id, the job can be polled using the poll_job method which will return a prediction object upon completion. These methods are ideal for cases where the user would prefer to postpone polling to a later time.

VII. COMMAND LINE INTERFACE

Upon installation, the Python AFLOW-ML client provides a command line interface (CLI) titled aflow-ml. The CLI exposes all the functionality of the Python client and is targeted at users who are not familiar with Python or using REST APIs. To receive a prediction the path of the POSCAR 5 file is passed to the CLI as a positional argument. Additionally, the model type is specified via the --model flag:

```bash
aflow-ml test.poscar --model=plmf
```

By default, the CLI will output the results to the terminal. The default functionality is modified by the use of additional flags. For instance, results can be saved to an out file by use of the -s flag:

```bash
aflow-ml test.poscar --model=plmf -s
```

where the predicted results are saved to a file titled prediction.txt. Additional flags exist which provide various levels of customization such as specifying the predicted values to return or the format of the output. A list of each flag is found below. This list is also viewable from the CLI using the -h or --help flags.

A. CLI flags

- **Model**
  - *Flag.* -m or --model
  - *Description.* (Required) Specifies the model to use in the prediction.
  - *Example.*
    - `aflow-ml test.poscar --model=plmf`

- **Save**
  - *Flag.* -s or --save
  - *Description.* Saves the prediction to a file. If the out file is not specified contents are saved to a file named prediction.txt.
  - *Example.*
    - `aflow-ml test.poscar -m plmf -s`
Outfile
  - Flag. `--format`
  - Description. Specifies the path and name of the out file.
  - Example.
    ```bash
aflow-ml test.poscar -m plmf -s --outfile=prediction.txt
    ```

Format
  - Flag. `--format`
  - Description. Specifies the format of the out file. Currently, text and JSON are supported.
  - Example.
    ```bash
aflow-ml test.poscar -m plmf -s --format=JSON
    ```

Fields
  - Flag. `--fields`
  - Description. State the predicted fields to show in the output. Expects fields as a comma separated list. If the flag is not present, all fields will be shown.
  - Example.
    ```bash
aflow-ml test.poscar -m plmf -s --fields=egap_ml,egap_type_ml
    ```

Verbose
  - Flag. `-v` or `--verbose`
  - Description. Toggle verbose mode. When enabled the CLI will log the progress of the prediction.

VIII. CONCLUSION

AFLOW-ML enhances materials discovery by providing streamlined open access to predictive models. The REST API promotes resource sharing, where any application, workflow or website may leverage our models. Additionally, the Python client provides a closed solution, which requires little programming knowledge to get started. With this flexibility, AFLOW-ML presents the accessible option for machine learning in the materials design community.

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