The AFLOW Fleet for Materials Discovery

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The traditional paradigm for materials discovery has been recently expanded to incorporate substantial data driven research. With the intent to accelerate the development and the deployment of new technologies, the AFLOW Fleet for computational materials design automates high-throughput first principles calculations, and provides tools for data verification and dissemination for a broad community of users. AFLOW incorporates different computational modules to robustly determine thermodynamic stability, electronic band structures, vibrational dispersions, thermo-mechanical properties and more. The AFLOW data repository is publicly accessible online at aflow.org, with more than 1.7 million materials entries and a panoply of queryable computed properties. Tools to programmatically search and process the data, as well as to perform online machine learning predictions, are also available.

I. INTRODUCTION

The AFLOW Fleet is an integrated software infrastructure for automated materials design [1] centered around the Automatic Flow (AFLOW) [2] framework for computational materials science. It features multiple scientific software packages, including the AFLOW high-throughput framework, the AFLOWP [3] medium-throughput framework, and the PAOFLOW [4] utility for electronic structure analysis, along with the AFLOW.org data repository [5]; its associated representational state transfer application programming interface (REST-API) [6], and the AFXUX Search-API [7]. These elements are well integrated with one another: a Python+JSON (JavaScript Object Notation) interface connects AFLOW, AFLOWP and PAOFLOW; and all software packages access the AFLOW.org repository via the REST-API and the Search-API.

Similar infrastructure has been developed by initiatives such as the Materials Project [8], NoMaD [9], OQMD [10], the Computational Materials Repository [11], and AiiDA [12]. The Materials Project uses the pymatgen [13] Python-language data generation software infrastructure, and their repository is available at materialsproject.org. The Novel Materials Discovery (NoMaD) Laboratory maintain an aggregate repository available at nomad-repository.eu, incorporating data generated by other frameworks including AFLOW. The Open Quantum Materials Database (OQMD) [10] uses tools such as qmpy to generate their database, which can be accessed at oqmd.org. The Atomic Simulation Environment (ASE) [14] is used to generate the Computational Materials Repository, available at cmr.fysik.dtu.dk. The ASE scripting interface is also used by the Automated Interactive Infrastructure and Database (AiiDA) framework available at aida.net, which revolves around relational databases for its overall design and data storage. Additional materials design utilities include the High-Toolkit...
II. AFLOW: EFFICIENT DATA GENERATION

The AFLOW framework for computational materials science automates the full workflow for materials properties calculations [2]. Using a standard set of calculation parameters [31], input files are automatically generated for the VASP [15, 16] DFT software package with projector-augmented-wave pseudopotentials [32] and the PBE parameterization of the generalized gradient approximation to the exchange-correlation functional [33]. Calculations are monitored as they run to detect and correct for errors without the need for any user intervention. Useful materials data is then extracted and processed for dissemination through the AFLOW.org repository. The entire framework is written in the C++ programming language (more than highly integrated 400,000 lines, as of version 3.1.153), providing a robust platform for continuous infrastructure development with reliable high performance.

A. AFLOW: Automated Workflows

AFLOW offers several automated workflows, each dedicated to a specific type of characterization yielding a set materials properties. For electronic properties, AFLOW performs four DFT calculations: two rounds of geometry relaxation (stage name: “RELAX”) using the VASP conjugate gradient optimization algorithm, a static run (i.e., fixed geometry; stage name: “STATIC”) with a denser k-point mesh to obtain an accurate density of states, and a band structure calculation (stage name: “BANDS”) following the AFLOW Standard path through the high-symmetry k-points in the Brillouin Zone [34].

Other workflows in AFLOW manage ensembles of DFT calculations, all offering the same automated error-correction procedures for high-throughput processing. For thermal and elastic properties, the Debeye-Grüneisen model (Automatic Gibbs Library, AGL) [35] is combined with the Automatic Elasticity Library (AEL) [36] as described in Section II F. A more accurate thermal characterization can be resolved with the finite displacement method for phonon calculations (Automatic Phonon Library, APL) [37] and its associated extensions, i.e., the quasi-harmonic approximation (QHA-APL) [38], as described in Section II G. AFLOW also extends beyond ideal crystalline materials characterization, offering modules to investigate off-stoichiometric materials (AFLow-POCC, Section II E) [39] and to predict metallic glass formation as a function of composition [19].

B. AFLOW: Prototype Library

The AFLOW framework uses decorated crystal structure prototypes for materials discovery [40]. Structural prototypes are specific arrangements of atoms which are commonly observed in nature, such as the rocksalt, zincblende and wurtzite structures. The atomic sites in these prototypes are populated with different elemental species to generate materials structures, for which the properties and thermodynamic stability are then obtained from DFT calculations. An extensive list of the structural prototypes included in AFLOW has been published in Ref. 40 and is available online at http://aflow.org/CrystalDatabase.

Pages within the website display a curated list of data for each structural prototype, including materials exhibiting this structure, various symmetry descriptions, the primitive and atomic basis vectors, and original references where the structure was observed. Accompanying these descriptions is an interactive Jmol visualization of the prototype, as described in Section II H. The page also contains a prototype generator, where the structural degree(s) of freedom and atomic species are defined to create new materials by leveraging the AFLOW prototypes module. This generates the corresponding input file for one of many ab initio software packages, including VASP [15, 16], QUANTUM ESPRESSO [17, 18], ABINIT [41], and FHI-AIMS [42].

C. AFLOW-SYM: Symmetry Analyzer

The AFLOW framework automatically analyzes the symmetry of materials structures, and returns a complete symmetry description. To address numerical tolerance issues, AFLOW employs an atom mapping procedure that is reliable even for non-orthogonal unit cells, and uses an adap-
Visualization of tolerance-sphere warping and adaptive tolerance method.

(a) Illustration of the warping of space when transforming from cartesian to fractional coordinates in the general case. (b) Spectrum of space groups identified by AFLOW-SYM with different tolerance choices.

Given a particular tolerance value, different symmetry operations can be realized in or excluded from the description of a crystal. Figure 1(b) highlights how the tolerance value affects the possible space groups for AgBr (ICSD #56551 with a reported space group #11). The neighboring space group regions are consistent with non-isomorphic subgroup relations, namely between space groups #59 and #11 and between #225 and #166. However, a gap or "confusion" tolerance region occurs between space groups #59 and #166 (with no direct subgroup relations). The problematic regions stem from noise in the structural data, impeding the identification of operations consistent with symmetry principles. This problem is solved by using a radial tolerance scan extending from the input tolerance $\epsilon_0$. Given a change in tolerance, the algorithm recalculates and verifies all symmetry properties until a globally consistent description is identified.

Aflow-Sym is compatible with many established ab initio input files, including those for VASP [16], Quantum ESPRESSO [17, 18], ABINIT [41], and FHI-aims [42]. From the structural information, AFLOW-SYM delivers the symmetries of the lattice, crystal (lattice + atoms), reciprocal lattice, superlattice (equally decorated sites), and crystal-spin (lattice + atoms + magnetic moment). This affords a multitude of symmetry descriptions to be presented, such as the space group number/symbol(s), Pearson symbol, point group symbol(s), Wyckoff positions, and Bravais lattice type/variation [34]. Moreover, the operators of the different symmetry groups — including the point groups, factor groups, space group, and site symmetries — are provided to users in rotation matrix, axis-angle, matrix generator, and quaternion representations for easy manipulation. All symmetry functions support the option to output in JSON format. This allows AFLOW-SYM to be leveraged from other programming languages such as Java, Go, Ruby, Julia and Python — facilitating the incorporation of AFLOW-SYM into numerous applications and workflows.

D. AFLOW-HULL: Convex Hull Analysis

Structure and energy data from the AFLOW.org repository are used to resolve the low-temperature/low-pressure thermodynamic stability of compound systems. For a given stoichiometry, the AFLOW.org repository provides the DFT energies of various crystal polymorphs. By exploring representative structures over the full range of stoichiometries, AFLOW-HULL constructs the minimum energy surface, i.e., the lower-half convex hull [44], defining thermodynamic stability for the system (at zero temperature and pressure). Structures on the hull are thermodynamically stable (ground state), while those far from the hull will decompose into a combination of stable phases, dictating synthesizability at these conditions. Any analysis of the hull requires sufficient statistics to ensure convergence, i.e., enough representative structures have been included in the alloy system calculations such that any additional entries are not expected to change the minimum energy surface.

The geometric construction offers several key properties critical for synthesizability. For a specific composition, the energetic distance to the hull quantifies the energy released during the decomposition, while the ground state phases defining the tie-line/facet below the compound are the products of the reaction. The distance from the hull also measures the “severity” of instability, i.e., structures near the hull may stabilize at higher temperatures or pres-
FIG. 2. Example convex hull illustrations offered by AFLOW. (a) 2D convex hull of the CuZr system generated automatically by AFLOW. (b) 3D convex hull of the CuMnZn system presented through the AFLOW-HULL application online: http://aflow.org/aflow-hull.

E. AFLOW-POCC: Partial Occupations

The AFLOW Partial Occupation module (AFLOW-POCC) [39] models configurational and structural disorder including substitutions, vacancies, and random lattice site occupation, by generating a set of representative configurations. First, a supercell size is determined that accommodates the fractional stoichiometry to within a user-defined tolerance. Given the supercell size, \( n \), superlattices are generated using Hermite Normal Form matrices [45], which are then decorated in accordance with the stoichiometry to generate all possible configurations, as illustrated in Figure 3. Duplicate configurations are rapidly identified and eliminated by estimating the energy of each structure using the Universal Force Field (UFF) model [46].
average employs a Boltzmann distribution weight which is
a function of a disorder parameter (temperature), energy
relative to the ground state configuration, and degeneracy
as determined by the UFF model. Ensemble-average prop-
erties are obtained relative to the ground state configuration, and degeneracy
as a function of a disorder parameter (temperature), energy
which is characterized by AFLOW and VASP, and are ensemble-averaged to resolve the system-wide properties.

F. AEL and AGL: Thermo-mechanical Properties

The AFLOW Automatic Elasticity Library (AFLOW-AEL [36]) and the AFLOW Automatic GIBBS Library (AFLOW-AGL [35]) modules determine thermo-mechanical materials properties from calculations of strained primitive cells. These methods are generally computationally less costly than the phonon (APL and AAPL) calculations described in Section II.G, although APL and AAPL generally give more quantitatively accurate results, particularly for properties where anharmonic effects are important. AEL and AGL have been combined into a single automated workflow, which has been used to calculate the thermo-mechanical properties for over 5000 materials in the AFLOW repository.

The AEL module applies a set of independent normal and shear strains to the primitive cell of a material [36, 47] as depicted in Figure 4(a), and uses DFT to calculate the resulting stress tensors. This set of strain-stress data is used to generate the elastic stiffness tensor, i.e. the elastic constants:

\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{12}
\end{pmatrix} =
\begin{pmatrix}
\epsilon_{11} & \epsilon_{12} & \epsilon_{13} & \epsilon_{14} & \epsilon_{15} & \epsilon_{16} \\
\epsilon_{12} & \epsilon_{22} & \epsilon_{23} & \epsilon_{24} & \epsilon_{25} & \epsilon_{26} \\
\epsilon_{13} & \epsilon_{23} & \epsilon_{33} & \epsilon_{34} & \epsilon_{35} & \epsilon_{36} \\
\epsilon_{14} & \epsilon_{24} & \epsilon_{34} & \epsilon_{44} & \epsilon_{45} & \epsilon_{46} \\
\epsilon_{15} & \epsilon_{25} & \epsilon_{35} & \epsilon_{45} & \epsilon_{55} & \epsilon_{56} \\
\epsilon_{16} & \epsilon_{26} & \epsilon_{36} & \epsilon_{46} & \epsilon_{56} & \epsilon_{66}
\end{pmatrix}
\]

written in the 6 × 6 Voigt notation using the mapping [48]:

\[
\begin{aligned}
11 & \rightarrow 1, \\
22 & \rightarrow 2, \\
33 & \rightarrow 3, \\
23 & \rightarrow 4, \\
13 & \rightarrow 5, \\
12 & \rightarrow 6.
\end{aligned}
\]

These elastic constants are combined to calculate the bulk, \(B\), and shear, \(G\), elastic moduli in the Voigt, Reuss, and Voigt-Reuss-Hill (VRH, \(B_{\text{VRH}}\) and \(G_{\text{VRH}}\)) approximations.

The Poisson ratio \(\nu\) is then given by:

\[
\nu = \frac{3B_{\text{VRH}} - 2G_{\text{VRH}}}{6B_{\text{VRH}} + 2G_{\text{VRH}}}. \tag{2}
\]

The AGL module is based on the GIBBS [49, 50] quasi-harmonic Debye-Grüneisen model, and calculates the energy as a function of volume, \(E(V)\), for a set of isotropically compressed and expanded strains of the primitive cell, as illustrated in Figure 4(b). The energy as a function of volume \(E(V)\) data are fitted by either a numerical polynomial or an empirical equation of state to obtain the adiabatic bulk modulus \(B_a(V)\), as shown in Figure 4(c). The Debye temperature \(\theta_D(V)\) as a function of volume is then calculated using the expression:

\[
\theta_D = \frac{\hbar}{k_B} [6\pi^2V^{1/2}n]^{1/3} f(\nu) \sqrt{\frac{B_a}{M}}, \tag{3}
\]

where \(n\) is the number of atoms per unit cell, \(M\) is the unit cell mass, and \(f(\nu)\) is a function of the Poisson ratio \(\nu\):

\[
f(\nu) = \left\{ 3 \left[ 2 \left( \frac{2}{3} \cdot \frac{1}{1-2\nu} \right)^{3/2} + \left( \frac{1}{3} \cdot \frac{1}{1-\nu} \right)^{3/2} \right]^{-1} \right\}^{1/2}, \tag{4}
\]

where \(\nu\) can be obtained from Equation 2 using AEL, or set directly by the user. The vibrational contribution to the free energy, \(F_{\text{vib}}\), is given by:

\[
F_{\text{vib}}(\theta_D; T) = nk_bT \left[ \frac{9\theta_D}{8T} + 3 \log \left( 1 - e^{-\theta_D/T} \right) - D \left( \frac{\theta_D}{T} \right) \right], \tag{5}
\]

where \(D(\theta_D/T)\) is the Debye integral:

\[
D(\theta_D/T) = 3 \left[ \frac{T}{\theta_D} \right]^3 \int_0^{\theta_D/T} \frac{x^3}{e^x - 1} dx. \tag{6}
\]

The Gibbs free energy is obtained from:

\[
G(V; p, T) = E_{\text{DFT}}(V) + F_{\text{vib}}(\theta_D(V); T) + pV. \tag{7}
\]

The volume which minimizes \(G(V; p, T)\) at a given pressure \(p\) and temperature \(T\) is the equilibrium volume \(V_{\text{eq}}\), which

![FIG. 3. Structure enumeration for off-stoichiometric materials modeling.](image-url)
is used to evaluate $\theta_0(V_{eq})$ and the Grüneisen parameter $\gamma$ as defined by:

$$\gamma = -\frac{\partial \log(\theta_0(V))}{\partial \log V}.$$  \hfill (8)

Finally, $\theta_0$ and $\gamma$ are used to calculate other thermal properties including $C_v$, $C_p$, $\alpha_v$ and $\kappa_L$ [35, 49].

**G. AFLOW-APL: Phonons**

The AFLOW Automatic Phonon Library (AFLOW-APL) [2] calculates the harmonic vibrational properties of a crystal using the finite displacement method. Computed properties include the phonon dispersion and density of states, vibrational entropy ($S_{vib}$), and the heat capacity (at constant volume, $C_V$) as a function of temperature. These features are determined through an analysis of the phonon modes, accessed through the Interatomic Force Constants (IFCs) [51]. To first approximation, the harmonic (second order) IFC $C_{i,j,\alpha,\beta}$ is the negative of the force exerted in the $\alpha$ direction on the atom $i$ when the atom $j$ is displaced in the $\beta$ direction, with all other atoms maintaining their equilibrium position. To determine the forces, the atoms of the structure (supercell) are individually perturbed as illustrated in Figure 4(d). The forces are obtained with DFT from the derivative of the total energy using the Hellmann-Feynman theorem. Supercells are used to sufficiently cap-
ture distortion two atoms in a supercell structure at a time as depicted in Figure 4(e), and then calculating the change in forces on the other atoms [38]. These IFCs are used to calculate the three-phonon scattering rates, and thus the scattering time and mean free displacement. These quantities are combined with the group velocities obtained from harmonic API to solve the Boltzmann Transport Equation and calculate $\kappa_L$ with quantitative accuracy [38].

**H. AFLOW: Visualization Tools**

AFLOW leverages a panoply of visualization tools for materials data, including standard software such as gnuplot, latex, and xmgrace for plots of phonon dispersions, electronic band structures, electronic density of states, and convex hull visualization. These plots are served publicly through the AFLOW.org repository.

To visualize crystal structures, AFLOW employs the Jmol software, which has incorporated substantial functionality for AFLOW-specific application. The JSmol branch of the software powers the online crystal structure visualizations in the AFLOW.org repository entry pages and AFLOW Prototype Library pages. With its recently added POSCAR reader, JSmol provides an assortment of capabilities ranging from different view perspectives, supercell expansions, and varying unit cell representations. A similar visualization application showing the AFLOW Standard high-symmetry paths in the Brillouin Zone [34] is currently being incorporated, as illustrated in Figure 5. Additionally, the Jmol desktop client offers a specialized macro (aflow) for visualization of alloy systems, which leverages the AFLUX Search-API.

**III. AFLOW$\pi$: MINIMALIST HIGH-THROUGHPUT**

The AFLOW$\pi$ [3] framework has been originally implemented as a minimalist software to perform verification tasks (see Section V G) on data published on AFLOW.org. By design, AFLOW$\pi$ is easy to install and to extend to a variety of electronic structure codes (currently only the QUANTUM ESPRESSO [17, 18] DFT package is implemented). AFLOW$\pi$ builds on the versatility of Python, providing a module to prepare, run, and analyze large sets of first principles calculations, and includes tools for the automatic projection on pseudo-atomic orbitals (PAO, see Section IV), and the self-consistent calculation of Hubbard $U$ corrections within the Agapito, Curtarolo and Bianconi Nardelli (ACBN0) approach [56, 57]. In addition, workflows for the calculation of elastic constants, diffusive transport coefficients, optical spectra and phonon dispersions with DFT+U (see Figure 6(a) for assessing the effect of the Hubbard $U$ corrections on the phonon dispersion calculated using APL). When possible, AFLOW$\pi$ exploits the tight-binding hamiltonians as in Ref. 58. Calculation results can be easily packaged and prepared for incorporation
exploiting the simplicity of the TB formalism and the efficiency of fast Fourier transforms, PAOFLOW interpolates the band structure and computes the matrix elements of the momentum operator, $p_{m,n}$. These are used to improve the quality of integrated quantities such as the density of states (adaptive smearing), to compute electronic transport coefficients within the constant relaxation time approximation, and to compute the dielectric constants \[58\]. In addition, the $p_{m,n}$ matrix elements facilitate the calculation of the Berry curvature and related properties (anomalous Hall conductivity, spin Hall conductivity; see Figure 6(b)), magnetic circular dichroism, spin circular dichroism; see spin texture of the nodal line and Weyl points in HfC shown in Figure 6(c)). Starting from a well interpolated band structure, it also possible to compute topological invariants.

Because of the local representation of the electronic structure provided by the PAOFLOW software, surface projected band structure and Landauer ballistic transport are also computable within PAOFLOW.

The software is implemented in Python, is portable and easy to install, and is parallel by design (on both CPUs and GPUs). PAOFLOW is also an integral part of the AFLOW\pi framework.

V. AFLOW: DATA REPOSITORY

The AFLOW data repository \[5\] contains the calculated properties for over 1.7 million materials entries, obtained using the AFLOW framework. These properties are available through the aflow.org web portal, which includes on-

FIG. 5. Side-by-size visualization of the crystal structure and Brillouin Zone using Jmol. The structure highlighted is Ag$_3$KS$_2$ (ICSD #73581): http://aflow.org/material.php?id=Ag6K2S4_ICSD_73581. The AFLOW Standard path of high-symmetry $k$-points is illustrated in the Brillouin Zone \[34\].

FIG. 4. Ensembles of distorted geometries for the calculation of thermo-mechanical properties with AFLOW. AEL uses the stresses from a set of (a) normal and shear strained cells to obtain the elastic constants. AGL calculates the energies of a set of (b) isotropically compressed and expanded unit cells, and (c) fits the resulting $E(V)$ data by a numerical polynomial or by an empirical equation of state. APL obtains the (d) second order harmonic IFCs from a set of single atom displacements and the (e) third order anharmonic IFCs from a set of 2-atom displacements.

IV. PAOFLOW: FAST CHARACTERIZATION

PAOFLOW \[4\] is a stand-alone tool to efficiently post-process standard DFT pseudo-potential plane-wave calculations to generate tight-binding (TB) hamiltonians which faithfully reproduce the calculated electronic structure (eigenvalues and eigenvectors) with arbitrary precision in reciprocal space \[59–61\] (see Figure 6(b) for PAOFLOW generated band structure for HfC (ICSD #169399, space group #187, AFLOW prototype: AB_hP2_187_d_a)). By

into the AFLOW.org data repository (see Section V).
FIG. 6. Vibrational spectrum calculated with AFLOWπ and AFLOW-APL (left) and electronic properties computed with PAOFLOW (right). (a) Phonon dispersion of CaF₂ calculated with APL [38], using the ACBN0 method as implemented within AFLOWπ (green lines). The results obtained using PBE are shown by the broken orange lines for comparison. The blue triangles and red unfilled squares represent neutron scattering data from Ref. 53 and Ref. 54 respectively, while the purple diamonds represent Raman and infrared data from Ref. 55. (b) Electronic band structure, spin Hall conductivity (SHC) and (c) spin texture of the nodal line and Weyl points in HfC, as calculated using the PAOFLOW utility.

line search/sort and data analysis applications. The repository is programmatically accessible through the AFLOW Data REST-API [6] and the AFLUX Search-API [7].

A. AFLOW: Web Portal

The AFLOW repository [5] is available online via the aflow.org web portal (Figure 7(a)). It contains multiple online applications for data access, processing and visualization, including the advanced “MendeLIB” search application at http://aflow.org/advanced.php which facilitates searching for materials entries with filters for elemental composition and calculated properties (see Figure 7(b)), the interactive convex hull application at http://aflow.org/aflow-hull (see Section II D), the online machine learning model at http://aflow.org/aflow-ml (see Section V B), and the AFLOW online tool at http://aflow.org/aflow_online.html which gives access to AFLOW crystal structure analysis and processing functions. These applications and more are accessible from the main aflow.org web page, via the “Apps and Docs” set of buttons highlighted by the dashed red rectangle in Figure 7(a).

B. AFLOW-ML: Online Machine Learning

The AFLOW machine learning (AFLOW-ML) online application provides a user interface to leverage machine-learning models trained on AFLOW data. It accepts a standard structure file (POSCAR or QE) and outputs predictions for properties such as the band gap, elastic moduli, heat capacity, Debye temperature, vibrational free energy, and thermal expansion coefficient. Additionally, structures within the AFLOW repository can be imported via the sidebar. This application provides an accessible medium to retrieve machine learning predictions without the need to install a software library or machine learning package.

Currently, AFLOW-ML supports two different machine-learning models. The first model, property-labeled materials fragments [30], plmf, has been trained using data from the AFLOW repository, and predicts properties such as the electronic band gap, specific heat capacities and bulk/shear moduli. The second method is the molar fraction descriptor model [62], mfd, which predicts vibrational properties such as vibrational free energy and entropy, and is based only on the chemical composition of the material.

The AFLOW-ML API [63] offers programmatic access to the AFLOW-ML online application, and provides a simplified abstraction that facilitates leveraging powerful machine learning models. This distills the prediction process down to its essence: from a structure file, return a prediction. Using the API is a two step process: first a structure file, in POSCAR 5 format (structure input for version 5 of VASP), is posted (i.e. uploaded) to the endpoint /<model>/prediction on the aflow.org server using standard HTTP libraries or dedicated programs such curl or wget, where <model> specifies the machine learning model to use in the prediction (current options: plmf and mfd). When a prediction is submitted, a JSON response object is returned that includes a task id. The results of the prediction are then retrieved from the /prediction/result/ endpoint on the aflow.org server by appending the task id to the end of the URL, i.e. /prediction/result/{id}/. This endpoint monitors the prediction task and responds with a JSON object that details its status. When complete, the endpoint responds
with the results of the prediction, represented as a JSON object containing a key-value pair for each predicted property.

C. AFLOW: Database Organization

The AFLOW data repository [5] is organized into project, set and calculation layers as illustrated in Figure 7(c). At the project layer, the calculations are divided into different catalogs based on the origin and composition of the entries [6, 7]. Within each catalog, entries are grouped into sets based on shared lattice type or alloy system. The entries within each set contain the results of DFT calculated properties for particular structures.

The AFLOW-ICSD catalog contains the DFT calculated properties for over 57,000 experimentally observed materials listed in the Inorganic Crystal Structure Database (ICSD) [64, 65]. Internally, this catalog is organized by lattice type, and then by individual materials entry. Since the materials in this catalog are already known to exist, the primary interest is in accurately calculating electronic structure and thermo-mechanical properties. Therefore, calculations for this catalog are generally performed using the Hubbard $U$ correction to the DFT exchange-correlation functional [66, 67] where appropriate, using a set of standardized $U$ values [31]. Within this catalog, entries are grouped by Bravais lattice type into 14 sets: “BCC”, “BCT”, “CUB”, “FCC”, “HEX”, “MCL”, “MCLC”, “ORC”, “ORCC”, “ORCF”, “RHL”, “TET” and “TRI”. The name of each materials entry is generated using the format <composition>_ICSD_<ICSD number>.

The entries in the other catalogs, such as “LIB1”, “LIB2”, and “LIB3”, are generated by decorating crystal structure prototypes to predict new hypothetical compounds, and contain unary, binary, and ternary materials, respectively. Additional catalogs, “LIB4”, “LIB5”, and “LIB6”, are currently being generated for quaternary, quinary, and hexenary materials. Within each catalog, the entries are grouped by element and exchange-correlation functional in the case of “LIB1”, and by alloy system in the cases of “LIB2” and “LIB3”. “LIB1” contains a total of 2784 entries, while “LIB2” currently has 329,181 entries and “LIB3” has over 1.3 million. Within each alloy system, the individual materials entries are named according the relevant crystal prototype. For these catalogs, the emphasis is on the discovery of new thermodynamically stable or metastable materials, and on their use to generate the thermodynamic density of states for the prediction of the formation of disordered materials such as metallic glasses [19] or high entropy alloys [24]. Therefore, calculations in these catalogs are performed using the GGA-PBE exchange-correlation functional [33] without Hubbard $U$ corrections [31] so as to produce consistent energy differences, enabling the calculation of accurate formation enthalpies.

D. AFLOW: Database Properties

Materials properties within the AFLOW repository [5] are indexed as keyword-value pairs which are programmatically accessible via the AFLOW Data REST-API [6] and programmatically searchable via the AFUX Search-API [7]. Search filters for these properties are also available in the advanced search application of the aflow.org web portal as highlighted by the dashed red rectangle in Figure 7(b), where they are grouped into chemistry (e.g., chemical species, stoichiometry), crystal (e.g., space group, Bravais lattice type), electronic (e.g., band gaps), thermodynamic (energetic and thermal properties, e.g., formation enthalpies and Debye temperatures), magnetic, scintillation, mechanical (elastic moduli and pressure-related properties), and calculation (e.g., k-point mesh, AFLOW version) parameters. In total there are in excess of 170 million individual materials properties indexed in the AFLOW database (~100 per materials entry). Lists of the keywords corresponding to the materials properties are provided in Refs. 6, 7, and 36.

Systems for which the “STATIC” and “BANDS” calculations have been performed are supplemented with automatically generated images of the density of states, projected density of states, and band structure. Both low (PNG) and high (EPS) quality variants of the images are available.
FIG. 8. Example band structure and density of states images automatically generated and served through the AFLOW.org data repository. The structure highlighted is AlCo$_2$Fe (ICSD #57607): http://aflow.org/material.php?id=Al1Co2Fe1_ICSD_57607. The results of the spin-polarized calculation are differentiated by: color on the band structure plot (black/red for majority/minority spin), and sign on the density of states plot (positive/negative for majority/minority spin). The band structure is calculated following the AFLOW Standard path of high-symmetry k-points [34].

for download. An example band structure and density of states image is displayed in Figure 8.

E. AFLOW: Data REST-API

The full data set generated by the high-throughput AFLOW process [5] is backed by a disk store of (at this time) over 12 TB of input criteria, calculated results, and derivative output. The backing store is exposed via the AFLOW Data REST-API [5] in a hierarchical organization. This direct exposure of our results not only grants the end user a high degree of utility via direct access, but more importantly, guarantees data provenance that promotes reproducibility. The hierarchy of the AFLOW Data REST-API categorizes this abundance of information into meaningful high-level classifications allowing for exploration of self-similar materials that are related by stoichiometric and/or crystallographic properties. Once a selection of materials has been determined, the full range of available properties and procedural data are retrievable.

The organizational hierarchy of both the underlying data store and the REST-API is project dependent, as described in Section VC. Each project is equivalent to one of the catalogs listed in Section VC, and in the REST-API are denoted by the project layers “ICSD_WEB”, “LIB1_RAW”, “LIB2_RAW”, and “LIB3_RAW”. Each project layer contains multiple set layers, which correspond to specific alloy systems in the case of “LIB1_RAW”, “LIB2_RAW”, and “LIB3_RAW”. For instance: http://aflowlib.duke.edu/AFLOWDATA/LIB2_RAW/ exposes the set layer for binary entries, where each set corresponds to different binary alloy system, allowing for pairwise atomic species examination. Within each set is the entry layer, consisting of decorated structural prototypes which provide stoichiometric and structural variation for each alloy system. Each entry contains the calculated results for a particular structure and composition, organized as keyword-value pairs. The calculated values of thermodynamical, mechanical, electronic, magnetic, chemical and crystallographic properties can be directly accessed by querying a Uniform Resource Identifier (URI) of the form <server>/<project>/<set>/<entry>/?<keyword>, where <server> is http://aflowlib.duke.edu/AFLOWDATA, <project> is the appropriate project layer, <set> is the alloy system, <entry> is the structural prototype, and <keyword> corresponds to the materials property of interest. A full description of the REST-API keywords is provided in Ref. 6, along with additions in the appendices of Refs. 7 and 36.

The ability to explore related entries predicated on a multitude of properties leads directly to novel materials discovery and use. The AFLOW Data REST-API disseminates our methods and results, without restriction, to a global research audience in order to promote scientific and engineering advancement.
F. AFLUX: Search-API

The Automatic Flow of LUX or AFLUX Search-API [7] is a human usable remote data search API. LUX is designed to be a domain agnostic solution to the outstanding problem of programmatically searching remote data that typically is either exposed via a capriciously limited utility or requires a-priori knowledge of the internal organization of the remote repository. The LUX query concept flattens the exposed data, while simultaneously providing arbitrarily complex query capability, allowing an end user full freedom in constraining the requested data. LUX is designed to operate in the nearly ubiquitous web URI context while minimizing any potentially conflicting interactions with existing URI functionality.

AFLUX is the domain specific implementation of LUX and is available at the <AFLUX-URI>: http://aflowlib.duke.edu/search/API/. At this time, the AFLUX API freely exposes over 170 million keyword-value properties, without any requirements or restrictions on the end user. Specific properties and compositions can be searched for by appending the appropriate keywords to the <AFLUX-URI>. Search results can be restricted by including specific values or value ranges in parentheses after the appropriate keyword. For example, a search can be restricted to entries that contain both of the elements Na and Cl, and have a calculated electronic band gap in excess of 1.0 eV, by including the search parameters species(Na,Cl), Egap(1,0+) in the query part of the URI. In LUX, “,” corresponds to the logical AND operator, and “*” is the loose operator which extends the search to entries in a specified value range. If no parameters are provided for a particular keyword, then the values of that property are returned for all entries which satisfy the remaining search criteria. A full list of all LUX logical operators can be found in Ref. 7, along with descriptions of their functionality and appropriate usage.

In addition to materials properties keywords, LUX also accepts directives, which behave as pseudo property keywords. They are used to provide additional information on LUX usage, and control the format and quantity of the returned data. Note that any directives included in a search query must come after all of the materials properties keywords. In particular, the schema directive can be used to retrieve the most current and canonical list of keywords using the AFLUX summons: <AFLUX-URI>schema,format(json).

G. AFLUX: Data Quality Control

Data quality control, including validation of methodolgies and verification of calculated data, is vital when constructing large databases such as the AFLUX repository [5] in order to guarantee the reliability of the results. Methodological validation involves quantifying the accuracy of calculation models with respect to experiment, while data verification includes checking the robustness of calculation parameters and the satisfaction of convergence criteria.

Physical models incorporated into the AFLOW framework are validated by comparison to benchmark sets of experimental data. This helps determine the predictive accuracy of the methods for real materials, as well as the regimes in which they are reliable. For example, the AEL and AGL modules were validated by comparison to a benchmark set of 75 experimentally well characterized compounds of various structural types [35, 36], and the accuracy was quantified by the Pearson and Spearman correlations, and the root-mean-square deviations. Similar validation analyses were performed for the QHA-API [37, 52] and AAPL methods [38], as well as the property labelled materials fragments machine learning model [30].

The AFLOW-PQCC methodology has been validated by comparing the band gap as a function of composition for ZnS$_{1-x}$Se$_x$ and Mg$_x$Zn$_{1-x}$O, and the magnetic moment per atom as a function of composition for Fe$_{1-x}$Cu$_x$, to experimental values [39].

The ACBN0 functional [56], implemented in AFLOW [see Section III] and PAOFLOW [see Section IV] has been validated by comparing the lattice parameters, bulk moduli, electronic band gaps, phonon modes, high frequency dielectric constants and Born effective changes it produces to the experimentally measured values for the Zn and Cd chalcogenides [68].

The convergence of both the charge density optimization and the ionic structural relaxation are automatically verified for all AFLOW calculations prior to incorporation into the data repository. This includes, for example, checking that the charge density has converged in accordance with the AFLOW standard settings [31], and verifying the relaxation of the cell size and shape by ensuring that all elements of the stress tensor are less than 10 kbar. The convergence level for any individual calculation can be verified by querying appropriate keywords for the stress tensor: stress_tensor, Pulay stress: Pulay_stress, residual external pressure on the relaxed cell: pressure_residual, and the $\delta E$ value for the final electronic convergence step: delta_electronic_energy_convergence, using the AFLOW Data REST-API [6] or the AFLUX Search-API [7]. Initial calculation parameters can similarly be obtained using the appropriate keywords, such as the k-point grid: kpoints, or the electronic energy convergence threshold: delta_electronic_energy_threshold.

CONCLUSION

The AFLOW Fleet for computational materials design automates first principles calculations of materials properties. AFLOW incorporates a wide range of different modules, including applications for symmetry and thermodynamic stability analysis, generation of ordered and disordered materials structures, and calculation of thermomechanical properties, in a single integrated framework.

AFLOW$\pi$ is a versatile minimalist framework that includes tools for projection onto pseudo-atomic orbitals (PAO) and the self-consistent calculation of Hubbard $U$ corrections us-
ing ACBN0. PAOFLOW generates tight-binding hamiltonians which reproduce the electronic structure calculated using first principles methods, facilitating the rapid calculation of electronic and magnetic properties such as transport coefficients and the Berry curvature. All results are stored in, and disseminated through, the AFLOW data repository, which is available online at aflow.org, and is programmatically accessible via the AFLOW Data REST-API and the AFlUX Search-API.

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