

materials**soundmusic**: a computer-aided data-driven composition environment for the sonification and dramatization of scientific data streams

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ABSTRACT

*materials**soundmusic** is a new computer-aided data-driven composition environment based on the sonification and remix of scientific data streams. Sonification of scientific data, i.e. the perceptualization of information through acoustic means, not only provides a useful alternative and complement to visual data representation, but provides also the raw data for potential artistic remixes and further musical interpretation.*

1. INTRODUCTION

What would it be like to walk among the atoms that form a crystal or weave through the electrons in their relentless dance inside a material? With the **materials**soundmusic**** project we want to answer this question by providing, on one hand, a data analysis and mining tool for the scientific exploration of large data systems, and on the other, by engaging the general public in the understanding and appreciation of materials through the enjoyment of sound, music and art. Two approaches are in common use for extracting new information from data: one is statistical analysis; the other is data perceptualisation, i.e. making data properties perceptible to the human senses. This is most notably achieved through the visualization of properties through graphs, which is so much an integral part of the scientific process that we rarely question how accurately and adequately visual representations help us understand the correlations among data. Sonification, the representation of data by acoustic means, is a potentially useful alternative and complement to visual approaches that has been explored only in a handful of cases and has never been considered in the realms of materials databases. Materials property databases are of enormous scientific and technological value because they provide the materials scientist with complete compilations of materials properties that can be used for materials discovery,

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development and rational design. Notwithstanding the impact of materials databases in research and industry, the connection with the general public is quite feeble, and these projects are not receiving the interest and engagement that they deserve. We are familiar with the intricacies and vastness of the universe but we give little thought to the universe of processes that happen constantly inside the materials that surround us and on which we depend in our everyday lives. Part of the reason is that over millennia we have developed a familiarity with celestial objects, seen as obeying mathematical and musical laws [1], and we have embodied a synergy between the scientific and artistic interpretation of this aspect of the physical world. A similar concept has never existed for the world of materials.

materialssoundmusic**** is meant to exploit the dual aspect of data sonification, the analytic and the artistic, and provide open source software tools for a novel approach to the dialogue between perceptualization of scientific data and artistic creation: a new computer-aided data-driven composition (CADDCC) environment for the sonification, remix and artistic reinterpretation of materials property data as expressive media, available through the project web portal [www.materials**soundmusic**.com](http://www.materialssoundmusic.com).

2. THE PROJECT

2.1 High-throughput sonification of the materials data repository AFLOWLIB.

The **materials**soundmusic**** project starts with the sonification of the materials property data from the online computational materials science repository AFLOWLIB.[2] AFLOWLIB is an extensive (more than 900,000 entries and growing) repository of materials property data (phase-diagrams, electronic structure and magnetic properties to name a few) generated using the high-throughput computational framework AFLOW [3] and freely available on the website of the AFLOW research consortium at AFLOWLIB.org. AFLOWLIB can be mined a posteriori for various, a priori unanticipated, applications [4], and the recognition of such value has made projects like AFLOWLIB one of the pillars of the Materials Genome Initiative [5,6]. The initial process

of sonification provides an abstract representation of the data that can be used for navigation and data mining of the database on scientific grounds. From there, the data stream is open for elaboration as principal element of a data-driven compositional environment.

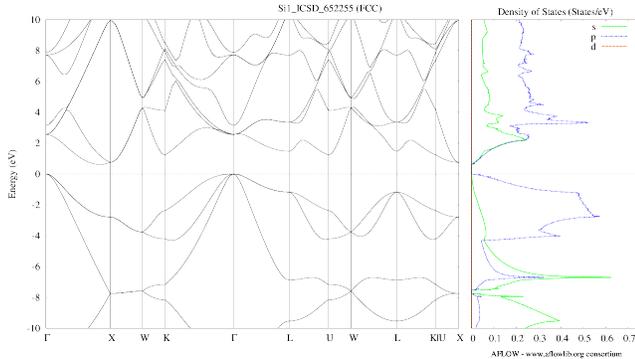


Figure 1. Band structure (left panel) and density of states histogram (right panel) of Silicon from the AFLOWLIB entry Si_ICSD_652255. Vertical axis is energy in eV eventually mapped onto MIDI notes; Horizontal axis: left panel - geometrical path in an auxiliary space eventually mapped into a timeline of events; right panel - histogram of the band structure (arbitrary units).

The first step in the sonification process is the identification of the property data that better ascertain the character of each individual material in AFLOWLIB. Among all possible choices, we opted for the sonification of the electronic band structure and of the density of states of a material. The electronic band structure of a solid describes those ranges of energy that an electron within the solid may have (called energy bands) and ranges of energy that it may not have (called band gaps) while the density of states measures the number of states per interval of energy that are available to be occupied by an electron (a sort of histogram of the electronic band structure). A visual representation of the data is displayed in Fig. 1.

2.2 The CADD environment

We have developed a sonification algorithm that can be easily embedded in the AFLOW framework in order to transform the density of state and electronic band structure data into sound material, by encoding energy data into MIDI events in an automated high-throughput fashion. The current algorithm maps energies in the range from -15eV to 5eV to the MIDI notes 21 through 108 (the 88 keys of the piano) and associates an amplitude (MIDI velocity) to each note according to the value of the density of states at that energy. The software tools for the CADD environment are based on Python, MAX[7] and Ableton Live[8]. We have developed a suite of Python scripts for the reading, mapping and formatting of the data: DATA2MIDI.py, which feeds a general-purpose app, the DataPlayer, that allows for sound synthesis and composition (see Sec. 2.4). Using DA-

TA2MIDI.py, data from the AFLOWLIB database are read and entries are mapped to MIDI events according to predefined algorithms where the choice of mapping can be made arbitrarily by the user. So far data can be mapped to MIDI notes from 21 to 108 on the full chromatic, diatonic, harmonic minor, diminished, whole tone and pentatonic scales or any 12 tone row of choice. DATA2MIDI.py is a script that accesses directly the database structure of AFLOWLIB and fishes the data for sonification. The script is run recursively for all the different entries and produces as output text files for each material (see Ref. [10] for a formal description of the database entries). This data mapping procedure is by no means limited to our particular choice of data. The algorithm is completely general and can be used on data from arbitrary sources: given a set of data [d] within an assigned numerical range [d_min,d_max] and a specific scale mapping on N notes, $scale(n)$, $n=0, \dots, N-1$ where $N = 88, 52, 36$, etc. for the chromatic, diatonic, pentatonic, etc. scale, respectively, and $scale(0)=21$ (A0) and $scale(N-1)=108$ (C8), the MIDI notes are simply obtained by:

$$MIDI_note(d) = scale(INT((d-d_{min}) * N / (d_{max}-d_{min}))),$$

where INT stands for the integer part of the number in parenthesis.

Similarly, we define a MIDI velocity in the range [0, 127] for each $MIDI_note(d)$ from the histogram of the data (density of state) for each data point, $HIST(d)$, with an appropriate normalization within an assigned range [H_min,H_max]:

$$MIDI_vel(d) = INT((HIST(d)-H_{min}) * 127 / (H_{max}-H_{min})).$$

2.3 The Data Sound Identifier

In the context of our materials data repository, we can use the fact that each material possesses a distinctive electronic signature to define a unique data sound identifier, or DSI, which fulfills the requirement of the sonification process for scientific data analysis. The DSI represents what in data sonification is called the *gist*, a short auditory message that conveys a sense of the overall trend or pattern of our data collection [9]. This process of sonification provides the user with an abstract representation of the data that can be used for navigation and data mining of the database on scientific grounds (for instance, materials with similar electronic band structure will have similar sonic signatures that can be used to filter database entries that can be suitable for specific classes of applications - as an auditory materials descriptor [3]). The encoding discussed in Section 2.2 is sufficient for producing a DSI based on the density of states, as discussed in Fig. 2, where we show four examples of DSIs for C (in the diamond structure), Si, Ge and β -Tin. It is extraordinary

how very similar DOS (such as for Si and Ge) have DSIs that are clearly distinguishable even for an untrained ear, demonstrating the power of the data encoding (see www.materialssoundmusic.com for the sounds collection).

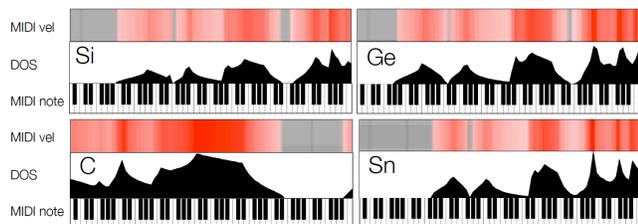


Figure 2. Density of states mapping for C (in the diamond structure), Si, Ge and β -Tin (data from the entries Si1_ICSD_652255, Ge1_ICSD_181071, C1_ICSD_52054 and Sn1_ICSD_53789 in AFLOWLIB). The sounds for the DSI can be heard at www.materialssoundmusic.com. In all the panels, the top row shows the MIDI velocity in shades of color (gray=0, red=127); the middle row shows the density of states data and their mapping on the 88 keys of the piano (MIDI notes 21 through 108).

2.4 Composition with data streams

All the files produced in the sonification of the AFLOWLIB database can be used as raw data for remix and further artistic/musical interpretation. In particular the band structure data with their intrinsically polyphonic character are ideal candidates for creating complex contrapuntal musical elaborations. While the energy mapping to MIDI notes is the same as in the DSI, the bands data provide us with a natural "timeline" of parallel events by the horizontal reading of the lines of Fig. 1 as individual musical voices. Here, each event in any voice, $d(t)$, is associated with a "duration time", τ , measured in terms of a `meter` unit specified in the DataPlayer app. In particular, the current algorithm infers the duration of each MIDI note-on-note-off events (that is a representation of rhythm and meter) from the rate of variation of the data (i.e. their derivative in time), making each material soundscape completely internally consistent: notes, velocities and durations are all an encoding of the data:

$$\text{MIDI_dur}(d(t)) = \text{meter} * \text{INT}(d(t) - d(t-1)),$$

with `meter` measured in milliseconds. Of course, other choices can be made arbitrarily during the composition process. The first compositional choice that one makes is clearly in the selection of the encoding: mapping the data to different scales or note patterns will create a different perception of the sound. From here, the composer can make use of any possible manipulation technique in order to promote his/her artistic vision. In the process, we are moving away from the pure sonification for scientific purposes and we enter the realm of individual artistic creation. Further manipulation can involve any functional composition tool that can be applied to the musical data (transposition, inversion, retrograde motion, multiplication, looping, randomization,

etc.) and can be done in a precomposed way or directly on the stream during the performance using common software (Excel, Numbers, MAX), scripting languages (awk, sed, python, java, etc.) or the suite of standalone MAX and MAX for Live patches (and VST plugins) through which the data stream is routed: the DataPlayer. A screenshot of the DataPlayer app and the schematics of its internal structure are discussed in Fig.3.

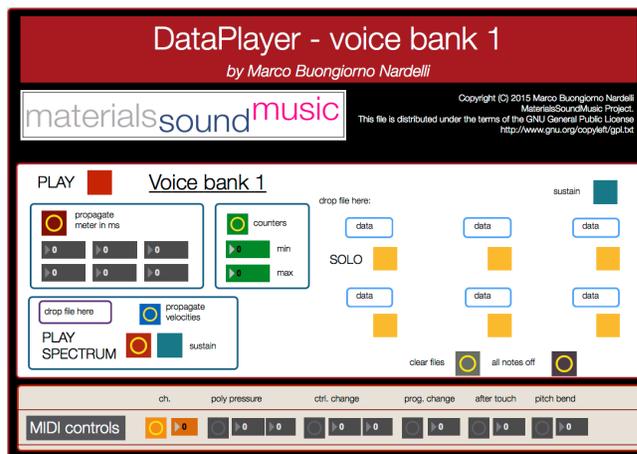


Figure 3. Screenshot (top) and schematics of the MAX/MSP patch internal structure (side): after the data file is assigned to the individual voice, `data2voice` reads the data (note, velocity and duration) sequentially using a `counter` controlled by the `meter` object; it then sends the stream to the `MIDIplayer` that encodes the data into MIDI events.

DataPlayer is typically integrated with Ableton Live as a MAX for Live MIDI plugin.¹

2.5 Notes on sonification mapping

The sonification of the scientific data is a compositional process that starts with the initial choices made by the scientist or composer: different mappings and encodings will produce different aural representations of the data that are in general uncorrelated and might enhance different characteristics of the data themselves. On one hand, this ambiguity has an artistic and compositional value that goes well beyond scientific analysis, on the other, the process would seem to lack the objectivity one needs for an effective data analysis for scientific applications. However, the introduction of the concept of a DSI generated using a common algorithm for all the data entries overcomes this difficulty and produces a coherent and consistent representation of the

¹ A standalone DataPlayer app for Mac can be downloaded at <http://www.materialssoundmusic.com/#!downloads/cik7>.

data. Provided that the same sound mapping is applied to all datasets, the sonification function remains valid, to a certain extent, also within the freedom of compositional decisions.

3. A MUSICAL EXAMPLE

The first example of a composition made with this CADD environment is *Music for 88 keys* by the author. A recording of it is available at www.materialssoundmusic.com [11]. *Music for 88 keys* is a suite born from the remix of the data from Diamond, Zinc Oxide and Gold. The piece is scored for player piano and electronics and is dedicated to the memory of Conlon Nancarrow, the American composer who made the player piano his instrument of choice throughout his career. In *Music for 88 keys* the original datasets from AFLOWLIB.org are variably manipulated through different techniques: from simple variations of tempo and meter to extensive reordering of pitches or regions and various orchestration choices. The suite starts with a *preludio* that uses the sonic mapping of the data for Diamond as starting compositional material. The same concept is used in the *interludio*, but with data from a different material, Zinc Oxide. *Interludio* separates the two principal sections of the suite: *largo* and *andante*, with the piano accompanied by sampled percussions sounds and based again on data from Diamond, from *continuo*, based on the data for Zinc Oxide for piano with a drone of brass, and *contrapunto aureo*, based on the data from Gold, where the brass and the percussions are both combined with the piano. The suite ends with a *postludio*, where the piano alone states again a sonic mapping of data that now combines the three materials.

4. CONCLUSIONS

With [materialsoundmusic](http://www.materialssoundmusic.com) we have created a computer-aided data-driven composition environment ideally suited for the sonification, remix and dramatization of scientific data streams. From the pure sonification of the data for scientific and data analytics purposes to the artistic manipulation of the information to create art music, we believe that this project will help promote and encourage a new level of engagement of the public with the world of materials and, in general, the advancement of all kind of collaborations and synergy between Computation, Science and Art.

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