

## Materials project database

The materials project is an open database that aims to mix the fourth paradigm of material science Engineering with the previous 3 methodologies to accelerate the process of discovering advanced materials and unravel their properties. The other important goal of this database is to make a platform that is open source which will enable an analysis of sophisticated materials. Material project is a core program of material genome initiative also known as MGI. Its main focus is to development of inorganic materials.

the first iteration was released on 28 February 2011 initially it was a root database that contains only the MIT database that has entries Inorganic Crystal database only. Then it was updated next month by removing the adjustment done for carbon, sulfur, Phosphorus, etc. the update on 10 October 2011 made it that data from the material genome website that was served before it is no longer supported.

The next major update to the database was on 13<sup>th</sup> April 2016 which saw major improvement. In this version, when the schema of data change minor version is the bump. A similar thing is done when new data is added.

The next major update to this database comes in November of 2018 which was considered a major overhaul of the software infrastructure. This enables a developer to continue to build new properties and be able to deliver them. In this update, many bugs were fixed, and certain development for infrastructure was done from scratch. Transparency was also increased to tell everyone the things that were changed and things that didn't change. It was decided that there will be monthly updates after V2018.11. this update also includes 5849 new materials ids. And 3556 retiring/re-aggregated materials ids.

The final major update was in 2019.05 in this update a new deprecated field to materials. This update makes it that by default its API searches only materials that are not deprecated.

Overall, 15,000 materials were deprecated, and 3,600 new materials. These deprecated materials will be recomputed to fill spaces back up.

The current database version is 2019.11

It has 3971 materials that are previously not added

Amorphous materials will have an amorphous tag.

Several inconsistency bugs for bandgap, elastic warnings, piezo tensors were fixed.

Materials project has three main pillars that are software's, supercomputer and screening

## Software:-

materials project is aiming to compute properties of all the known materials, this will enable it to remove the guesswork from the field of material design in several different uses. The data project also wants to data-mine new scientific trends in materials properties. This is done by providing information to the material researchers. This would let to overall faster innovation in the field of material research

## Supercomputers

National laboratories have supercomputing clusters that aim to provide the necessary infrastructure that lets algorithm and data computation to process at very high speed. Materials project use NERSC scientific computing center and its research division. And also OLCF, San Diego's SDSC.

## Screening

It shows the main benefit of the database because of advances in material science now we can predict properties of certain materials even before they are even synthesized. With the help of supercomputer clusters, many battery materials that are being tested in the lab are being predicted.

Materials project has open data and computational data and it doesn't have an expiration date. It uses several workflow management tools. And has a robust web-based API along with several Data analysis tools.

One of the challenges associated with DD- MSE that when such large datasets are created such as material projects they adhere to computational standards. So a certain standard has to be issued the material project is the leader in such standardization. The materials project has a very efficient distribution channel for the data is stored in it. The data is accessible about webpage which can be accessible by clients. The database has an open-source library that helps in the dispersal of large and rich materials and its aims that it should be accessible to all.

The material project is relevant to many applications python materials genomics library 58 it defines the core object of python in materials project. Pymtgen has an active member of 100 collaborators which led to an increase in its robustness. Currently, material API only supports unidirectional information transfer that would be from the database to the user. In the future API can be developed which will enable the user to transfer the data from his side to the database to increase the overall effectiveness of the database. Furthermore, a computational project of an individual user machine can be used to process supplement computation and automatic computation. This can lead to several discoveries in the future such as improvements in li-ion anodes, graphene, carbon nanotubes, etc.

Role in the Development of MUSE will be major as it will act as a backbone to expand in new areas. Materials ultimate search engine can use Materials project feature such as on-demand calculations. Cutting edge electronics etc.

## **NIST**

### **repository on interatomic potentials**

NIST repository on interatomic potential is a repository that provides a source that provides files related to interatomic potentials, it has evaluation tools that can be used to help the researcher in obtaining interatomic models and to judge the there respective quality and their applicability. The main difference developer is encouraged to enter new stuff that can contribute to further development. All materials and the different potential classes are allowed. material has an interatomic potential file or related file available in the repository. Such as conductors, semiconductors, oxides, etc.

The primary focus of NIST is on alloy, Coarse-Grained, and Fictional Potential

The NIST has around 148 multi-element systems and non-element material whose database is at Nist. Several multi-element may not have coarse-grained potentials data stored on NIST. Fictional potentials have been fitted purposefully to unrealistic target properties so they don't represent accurate real materials.

There is a method to submit new elements to the repository that is to send an email to [potentials@nist.gov](mailto:potentials@nist.gov). the national Institute of Standardization and technology admins prefer files to be received by the developer so that data integrity can be achieved.

Nist plays a very important role in the molecular simulation community. As it is forefront in data storage of molecular force fields. The good part about the NIST repository is stakeholders can participate in it if they knew its fundamentals. The NIST has lots of metadata that needs to be converted into valuable data that can be used by developers. The challenge with NIST is standardization as the different user can submit different data.

NIST coin Research

The goal of NIST and MGI are pretty much aligned. US innovation and industrial competitiveness are promoted by NIST and MGI wants to optimize this solution and make them practically feasible. The government as a stakeholder has got great benefit from NIST One of the best example is how research from NIST has enabled to bring down the cost of

manufacturing Nickels. Nickels are widely used as change in united states, earlier there manufacturing cost was not much but with gradual time there manufacturing cost has increased as nickel is used in other products.

The NIST research team has worked with US mint, the team from NIST has found a new approach for the production of nickel coin for cheap. The team approach cost of materials to produce nickel by 40%. Also, the new coin won't be fragile as compared to the older coin this can further help many tech companies to bring down the price of their electronics product which requires new resilient materials for their product. The coin making process is typically the coin should not corrode easily by an outside factor. Also, the engraving on the coin should be able to withstand years of wear and tear, plus there is the issue of counterfeit too.

The coin also should have electrical conductivity to a certain degree so that it can work in the vending machine.

The NIST Material Genome initiative was able to fulfill this demand as their goal is to bring the overall cost down of new material research. The government as a stakeholder of NIST can be seen to be getting a very big profit from it. The NIST repository is a file repository that accepts data in any format. To better handle data and increase searchability. The acceptance of metadata gives NIST to be a very important component of the MGI data infrastructure, and it will enable it to evolve further and help the Material genome initiative community as a whole.