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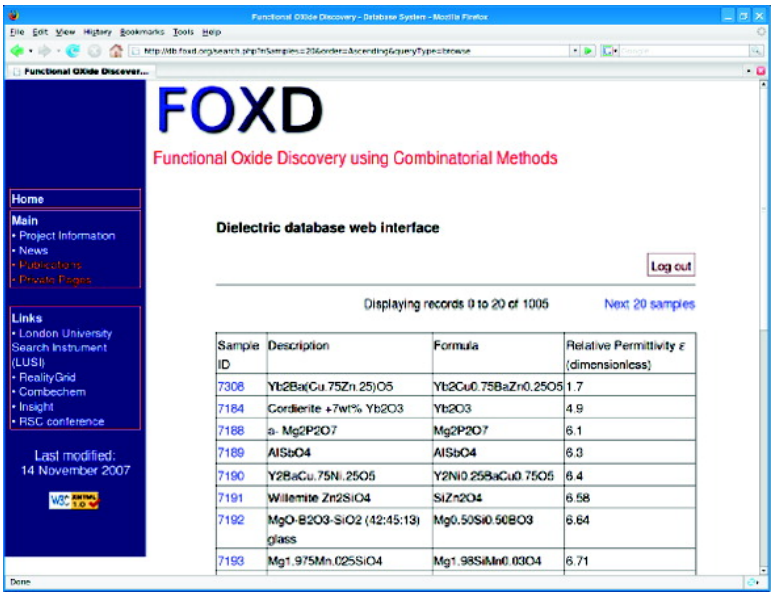

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Functional Ceramic Materials Database: An Online Resource for Materials Research

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We present work on the creation of a ceramic materials database which contains data gleaned from literature data sets as well as new data obtained from combinatorial experiments on the London University Search Instrument. At the time of this writing, the database contains data related to two main groups of materials, mainly in the perovskite family. Permittivity measurements of electroceramic materials are the first area of interest, while ion diffusion measurements of oxygen ion conductors are the second. The nature of the database design does not restrict the type of measurements which can be stored; as the available data increase, the database may become a generic, publicly available ceramic materials resource.

1. INTRODUCTION

There has been extensive work on the development of databases in combinatorial chemistry, and vast literature is available, particularly pertaining to the pharmaceutical industry.[1,2] In addition, previous work has investigated the combinatorial materials[3] and catalyst[4−6] optimization fields. Several materials databases are available, including the WebSCD (Structural Ceramics Database)[7] at the National Institute of Science and Technology (NIST),[8] the Dielectric Database Online[9] based at the University of Utah, and MatWeb,[10] a commercial materials database. WebSCD is heavily based in structural data and physical properties and there are very little data pertaining to functional properties such as dielectric and/or diffusion measurements. The Dielectric Database Online permits free text searches of a collection of literature pertaining to dielectric measurements and is heavily focused toward agriculture. MatWeb permits fine grained searching for a wide range of materials. However, the materials are limited to those manufactured by industry, and the database contains the data found in manufacturers' data sheets.

Consequently, a database providing a repository for materials which are currently investigated and reported only within the original literature would be an extremely valuable resource for the academic community. Extraction of compositional, synthesis, and property data permitting fine grained searches will provide substantial benefit to materials researchers. Previously, a materials database for fusion research has been developed;[11] our work builds on these efforts through the development of a ceramic materials database. The database system forms the foundation for data-mining tools which extract patterns and knowledge from the database, resulting in composition-structure-property relationships which are used to design new compounds. The data obtained from these new compounds can be used to improve predictive models,[12] and, through the execution of such *materials discovery cycles*,[13] we can iteratively improve materials designs.

We are currently involved in the Functional OXide Discovery (FOXD)[14] project, a pioneering combinatorial approach to materials discovery and materials research. The project is focused on two main classes of ceramic materials: dielectric materials for use in telecommunications and other electroceramics applications and oxygen diffusion materials which form components of solid oxide fuel cells (SOFC). Development of optimal materials for these applications is accomplished through the use of high-throughput combinatorial searches.[13,15] Combinatorial methods have the potential to generate vast quantities of data, and the discovery of materials design ideas requires the development of informatics and database systems[16] for management and analysis of these data.

Sample production for the FOXD project is performed using the London University Search Instrument (LUSI),[16] a combinatorial robot which combines an ink-jet printer and furnace for automated sample synthesis. The samples are created from mixtures of ceramic inks developed from milled powders.[17] The crystal structure of samples is verified using X-ray diffraction (XRD), and the dielectric properties of the samples are analyzed using scanning and contact measurements at kHz-GHz frequencies,[18,19] while ion diffusion properties of the samples are measured using Secondary Ion Mass Spectrometry (SIMS).[20] The microstructure of the samples is examined using scanning electron microscopy (SEM), and the composition is verified using energy dispersive X-ray spectroscopy (EDS).[18]

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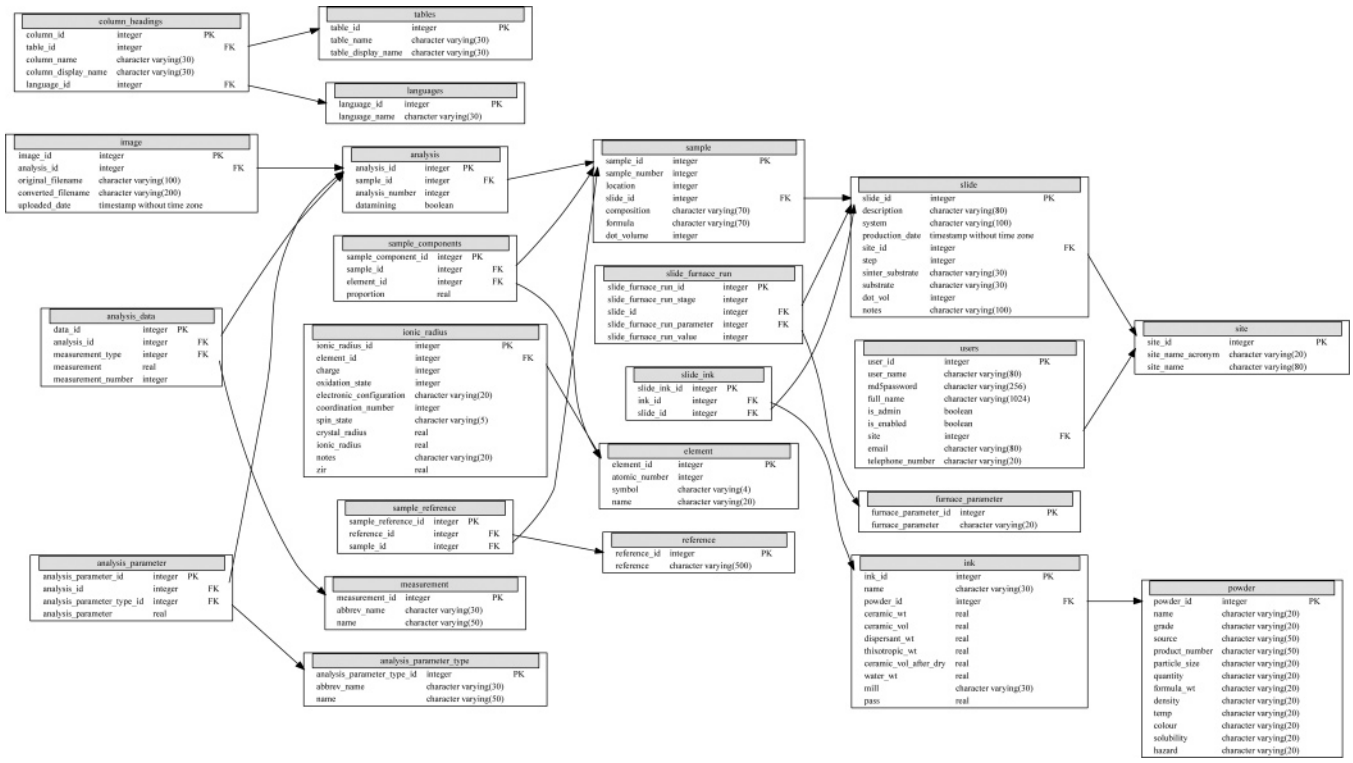


Figure 1. The structure of the database. The data are stored within the tables displayed. The table relationships are indicated by arrows.

2. DATABASE DESIGN

We have designed our ceramic materials database to handle a wide variety of experimental data. Currently, the database contains data produced by LUSI along with published data extracted from the literature. The generic database design permits data from other sources to be readily incorporated. The database stores sample production data, such as materials compositions and sintering temperatures, which are complemented by sample metadata including measurement method and measurement parameter data. In addition, the database can store images of samples, data files, and documents relating to experimental results. This central repository, accessible via a Web interface, enables geographically separate sites to have access to accurate, reliable, up-to-date information on sample production and measurement status and helps to eliminate the redundancy which would be found were each site to record its own data separately.[21] In addition, a single, complete database permits data-mining algorithms to operate on the complete data set, rather than on separate sections.

The OGSA-DAI project[22] aims to develop middleware to assist access and integration of distributed data sources. The use of OGSA-DAI might have been beneficial, had the project required the integration of initially distributed databases. However, since the project involved creating the database from scratch, the current centralized system provides the simplest solution.

2.1. Database Structure. The FOXD project uses the PostgreSQL[23] (http://www.postgresql.org/) database management system (DBMS) running on the Linux operating system. The database server is a virtualized system running on a 4-core AMD Opteron host. Virtualization permits transparent migration between physical systems. If performance requirements demand, the entire database can be transferred onto a more powerful system which occurs transparently to the end user.

The PostgreSQL DBMS is a powerful, open source, relational database system capable of handling the large quantities of data which are beginning to be generated by the FOXD project. A relational database is a collection of tables interconnected via relations. Data are created, retrieved, updated, and deleted using Structured Query Language (SQL), the standard language for database management. SQL was designed specifically to query data contained in a relational database and permits the building of complex queries.

The database schema is shown in Figure 1. Several tables contain data which are relevant to both sections (LUSI data and literature data) of the database, for example, element information such as atomic number and valency. The essential contents of the database are the tables containing compositional and property data for each particular material. The differences between the two data sets are found in the metadata. The literature data set contains metadata pertaining to the references from which the data are obtained, while the LUSI data set contains all of the sample production records, including a more detailed description of sample manufacture and sample measurement.

Various tables are used to store data such as sample compositions, library synthesis parameters, ink manufacturing details, ceramic powder information, sample location data, and even images associated with various stages of the manufacturing process. This database layout is available in more detail on the database Web site (section 4). Furthermore, by using tables to store details of, for example, measurement techniques and types of analysis data, extra measurements and parameters can be added without altering

the underlying design. This static design approach is important in database systems since it allows the database engine to store the data in the optimal fashion.

2.1.1. Literature and LUSI Data Sets. The literature data set contains composition and performance properties extracted from peer-reviewed journals and can be fitted into two broad categories: dielectric ceramic materials, with compositional information and permittivity measurements, and a data set of ion-diffusion materials and measurements. The database includes an index which relates each record back to its original article allowing users to determine the provenance of each record. The inclusion of this metadata is particularly important since different references often publish results on the same, or very similar, compositions.

In the case of the dielectric materials data set, the data was extracted manually, resulting in a spreadsheet containing columns for the chemical formula and property measurements. The diffusion data set was extracted partially by automatic methods. The "Digitize" V0.99 software package[24] authored by Dr. Danon was used to extract numerical values from graphical figures. For tabular data, manual methods were used, and the resulting data entered into a spreadsheet. Both the dielectric and diffusion spreadsheets were parsed using Perl[25] and inserted into the database. The Perl module "PerlMol"[26] was used to parse the string containing the chemical formula to extract the individual elements and quantities, permitting detailed compositional information to be recorded.

The LUSI data set contains production and analysis data for all of the samples synthesized by LUSI. It comprises details of the powders used to manufacture the inks as well as records of the ink production parameters. Automated ink mixing permits the generation of compositional ranges of samples which are printed onto the slides. The sintering and other manufacturing conditions of these slides are also recorded. At the time of writing, the materials under investigation are similar to those found in the literature data sets. As work progresses, however, the range of compositions in the database will broaden, increasing the generality.

2.1.2. Database Schema Design. In general, changes to the structure of the database should be avoided, once the system "goes live". It is therefore important that the database is designed such that new analyses, measurements, parameters, etc. can be added into the database without modification to the structure of the database. Analysis types, measurement types, and parameter names are recorded in individual tables, allowing addition of measurements simply through the addition of a record to the relevant table. "Pivot tables" are automatically generated tables which use rows from one table as column headings in another and can be used to dynamically generate tables containing a variable number of columns. In this way, when added to the measurement table a new measurement type will automatically appear as a column in the generated pivot table, permitting the addition of new analyses, measurements, and parameters without modification of the underlying database structure.

2.2. Database Access Interfaces. There are a number of interfaces available for access, depending on the needs of the user. The primary method of entering data is through the use of software written in Perl,[25] which parses templated spreadsheets, and the data are inserted into the database using SQL. A Web-based front end is also available. The system runs the Apache[27] Webserver software and employs the PHP[28] scripting language to connect to the database and execute SQL queries. The front end system allows users to obtain statistical information and permits data browsing, searching, and filtering using a variety of search methods (for example, according to composition, measurement values, and production date). This search functionality will become richer as the user-base requests more fine grained search and analysis capabilities. A screenshot of a Web page allowing users to browse through the dielectric data is shown in Figure 2.

Other access methods include the ability to directly connect to the database from within custom written C/C++ applications. This allows almost limitless application of a wide range of data-mining tools. An informatics system has been developed which allows users to enter production and experimental data quickly and efficiently;[16] this is immediately available for other users to access.[29,30]

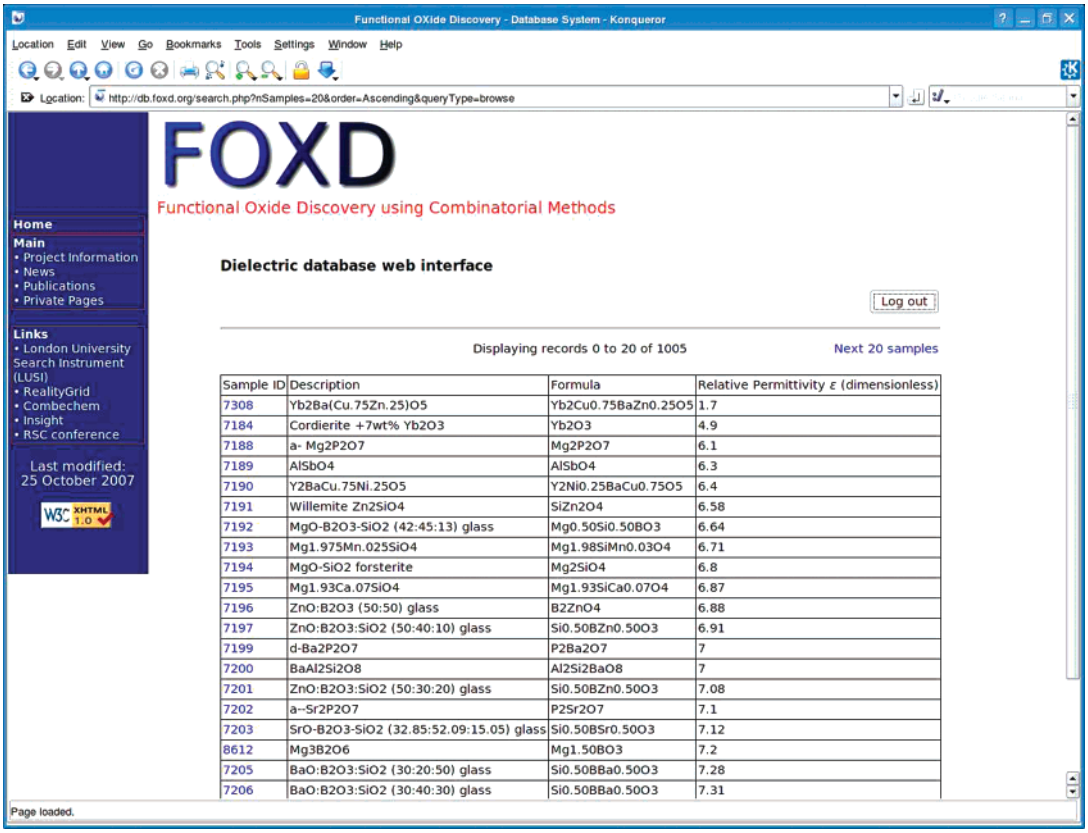
Currently, we require that external data submitted for inclusion in the database must be published in a peer-reviewed journal. This is used as a basic safety net to ensure data quality. Additionally, we are considering appointing "data managers" who will be responsible for particular data. For example, the data relating to dielectric properties will be assigned to a person who has the authority to approve or deny requests to add data when these are made. In this way, we can potentially accept data from unpublished sources, provided that the data manager is satisfied that the submitted data has been obtained using appropriate experimental methods and that the data is reliable.

Data modification is more problematic. Ideally, the reason for a discrepancy between two results will be contained within the experimental or measurement metadata, and so the results constitute two separate data points. In practice, there may be insufficient metadata available to determine the reason for the discrepancy, and so a decision must be made. In such situations, either we determine that one result is invalid or that both are valid and the difference can be explained by the experimental or measurement error. In the first case, we simply retain the correct data; in the second, we substitute the mean results. In both cases, the original data are retained for archival purposes.

Within the Web front end system, three categories of users are defined. The administrator has access to the complete database and can make system wide changes to the table structure and data. Other users have write access to the data and can make alterations to the data, but they cannot alter the table structure. Finally, read-only users can only read the data in the database, with no changes permitted. As mentioned previously, we are considering a fourth user category, "managers" who will have the ability to approve/deny data addition/modification requests and will be responsible for ensuring that the data contained within their section is accurate.

3. FEATURES AND APPLICATIONS

By making materials data available in a logically ordered, well-defined way, we are providing what we hope will be a valuable resource to the scientific community. The ability to browse through the data and to perform searches based



Sample ID	Description	Formula	Relative Permittivity ε (dimensionless)
7308	Yb2Ba(Cu.75Zn.25)O5	Yb2Cu0.75BaZn0.25O5	1.7
7184	Cordierite +7wt% Yb2O3	Yb2O3	4.9
7188	a- Mg2P2O7	Mg2P2O7	6.1
7189	AlSbO4	AlSbO4	6.3
7190	Y2BaCu.75Ni.25O5	Y2Ni0.25BaCu0.75O5	6.4
7191	Willemite Zn2SiO4	SiZn2O4	6.58
7192	MgO-B2O3-SiO2 (42:45:13) glass	Mg0.50Si0.50BO3	6.64
7193	Mg1.975Mn.025SiO4	Mg1.98SiMn0.03O4	6.71
7194	MgO-SiO2 forsterite	Mg2SiO4	6.8
7195	Mg1.93Ca.07SiO4	Mg1.93SiCa0.07O4	6.87
7196	ZnO:B2O3 (50:50) glass	B2ZnO4	6.88
7197	ZnO:B2O3:SiO2 (50:40:10) glass	Si0.50BZn0.50O3	6.91
7199	d-Ba2P2O7	P2Ba2O7	7
7200	BaAl2Si2O8	Al2Si2BaO8	7
7201	ZnO:B2O3:SiO2 (50:30:20) glass	Si0.50BZn0.50O3	7.08
7202	a--Sr2P2O7	P2Sr2O7	7.1
7203	SrO-B2O3-SiO2 (32.85:52.09:15.05) glass	Si0.50BSr0.50O3	7.12
8612	Mg3B2O6	Mg1.50BO3	7.2
7205	BaO:B2O3:SiO2 (30:20:50) glass	Si0.50BBa0.50O3	7.28
7206	BaO:B2O3:SiO2 (30:40:30) glass	Si0.50BBa0.50O3	7.31

Figure 2. The Web interface to the dielectric database. The page allows users to browse through the dielectric database and see the composition and permittivity of the materials in the database. Other pages which permit searching for particular permittivity values and elements are also available.

on properties and/or compositional information enables users to rapidly determine previous work completed and to identify "gaps" in current knowledge which will help to prevent duplication of effort.

Additionally, data mining algorithms can be applied to the data to yield important insights into composition-structure-property relationships.[31] To enable this ability, the user must be able to generate data sets using flexible record selection rules which are then exported from the database in a machine readable format.

3.1. User Requirements. In order to enable users to browse/search the available data and also to enable application of data mining algorithms, several requirements were identified. The user must be able to:

1. Browse through the whole data set. This view of the data permits the user to view the composition and property information for the records in the database.

2. Select records based on a range of properties. The system allows the user to enter a permittivity range which allows the user to select records which have a particular permittivity.

3. Select records based on their composition. Compositional information can be used to select records from the database. The system allows the user to enter a desired element and the quantity required.

The selected records are displayed on the screen as shown in Figure 2. When a user selects a particular record from this screen, another page is displayed. This screen provides further metadata and includes the original referenced publication from which the data was extracted.

To facilitate data mining of the selected data set, the data must be available in a machine readable format. Two main formats are available: In the first case, comma separated variables (CSV) are provided; in the second, XML based markup can be exported.

3.2. Data Mining and Visualization. One example of a data mining algorithm is the artificial neural network (ANN) which uses a data set extracted from the database to learn composition → function relationships. We have developed an ANN which allows users to make predictions of materials properties, such as permittivity and diffusion coefficient, using only the composition of the material.[32]

A Web-based interface to the ANN permittivity predictor has been developed and is also publicly available (Figure 3). To obtain property predictions, the user enters the material composition into a Web form which is then submitted to the prediction system. The ANN is executed, and the predicted result is returned to the user. Since the ANN is trained using data contained within the database, the predicted results are more likely to be accurate for materials which are similar to those found in the database. For example, oxygen is ubiquitous, whereas aluminum is only present in a few materials. Since the ANN will attempt a prediction for any entered material, statistics are generated from the database, along with a reliability index, to permit the user to make an informed decision about the accuracy of a prediction.

The Web-based ANN prediction system is provided via a Web service,[33] which provides a means for running applications over the Internet. The approach allows the separation

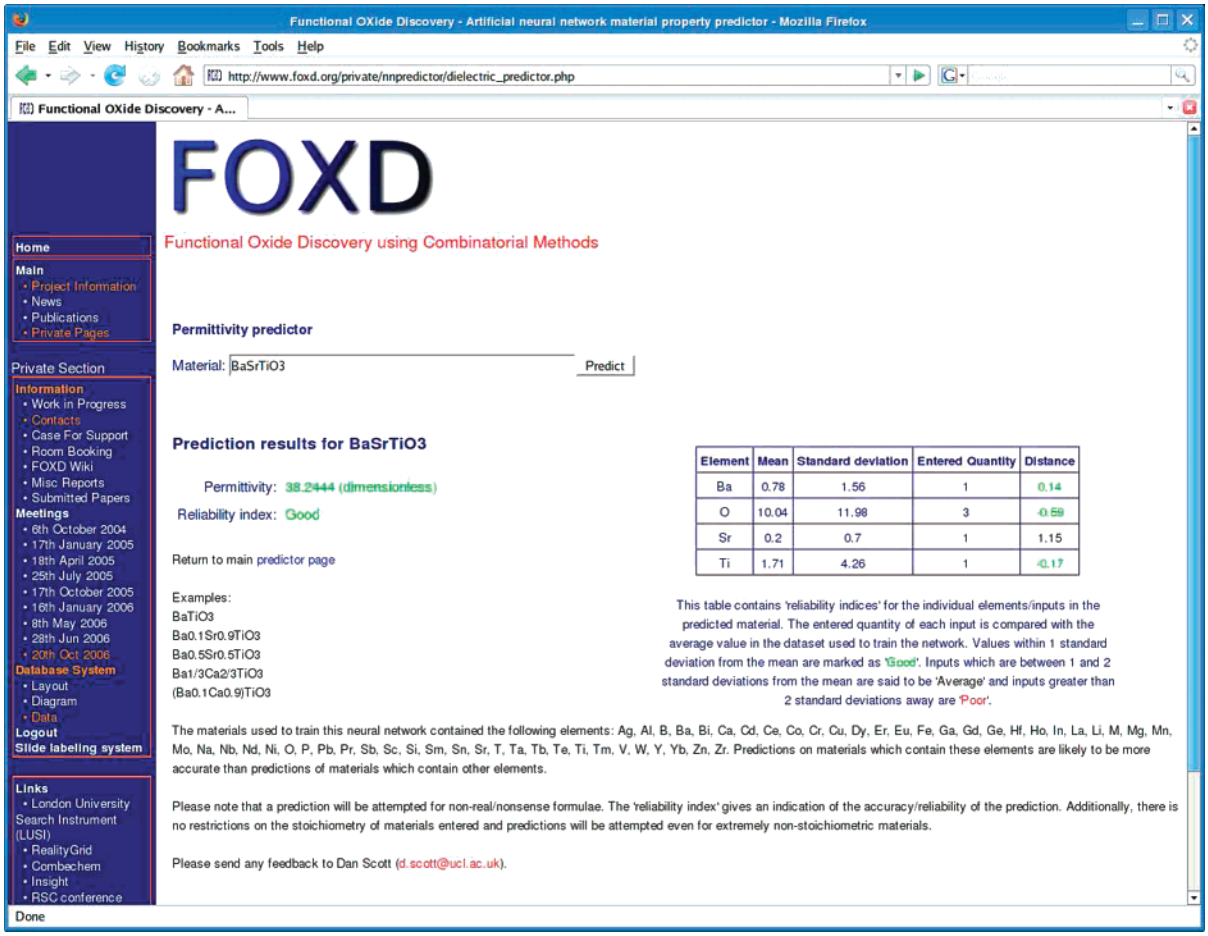


Figure 3. The Web interface to the neural network based dielectric predictor. By submitting materials compostions on this page, the user can obtain a predicion of the dielectric constant along with training data set statistics which permit the prediction reliability to be gauged.

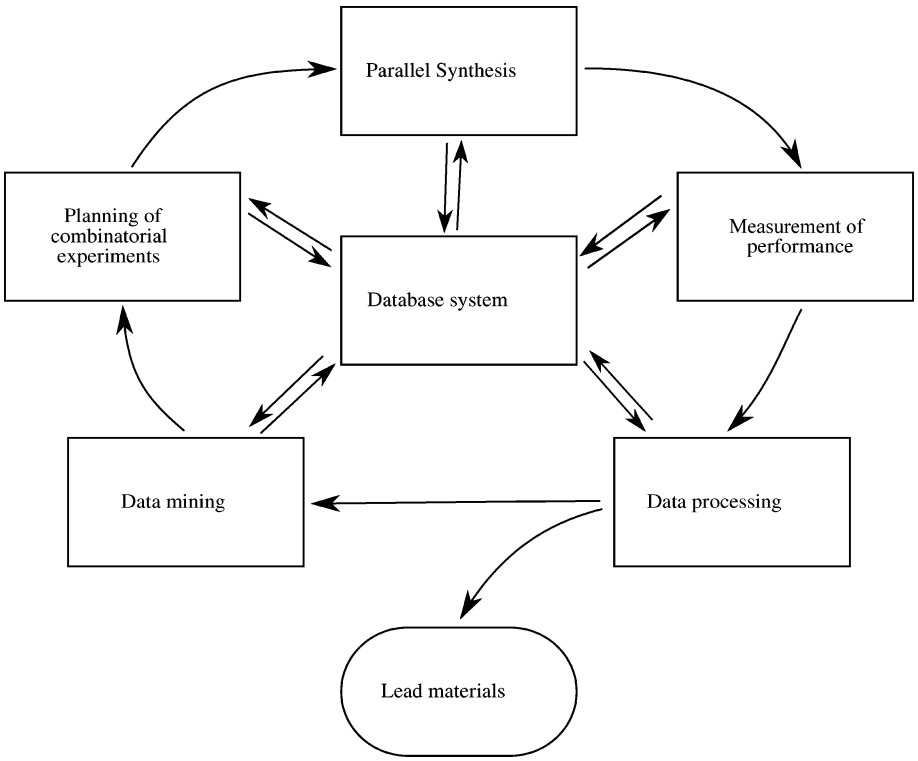


Figure 4. The combinatorial materials discovery cycle. The database forms the central 'hub' of the system.

of Web and application servers which is more flexible and secure than a monolithic system. This also means that CPU intensive applications such as ANN training and genetic algorithm materials design can be run on a suitable high

performance machine, freeing up the Web server. As the informatics system is used to add and update data, the ANN can automatically be retrained.

Apart from ANNs, classification algorithms such as Support Vector Machines (SVM)[34] can be used to predict other types of data. For example, the manufacturing conditions and processing of ceramic samples also affect the properties and quality of the final sample. Since ceramic processing conditions are recorded in the database, along with details of the sample condition, optimal conditions (sintering time, temperature, etc.) for the production of good samples can be determined.

3.3. Materials Design. There has been considerable work on the design of chemical compounds and materials using data-mining techniques, particularly in the pharmaceutical industry.[3,35,36,37] Catalyst design is also a popular area for materials design using data-mining techniques.[4,6,38,39] However, minimal work has been published on the design of ceramics with electronic and ionic conducting properties.

By applying a genetic algorithm to the ANN prediction algorithms, we have designed materials which are predicted to exhibit optimal properties.[40] The genetic algorithm employs stochastic search techniques to invert the ANN, thus providing predictions of materials suitable for laboratory examination. These predictions complete the materials discovery cycle shown in Figure 4 and are used to suggest materials for production by LUSI. By repeating this cycle, we can iteratively improve the materials designs until an optimal composition is obtained.

4. PUBLIC AVAILABILITY

The database is available for academic use, access details of which can be obtained from http://db.foxd.org. Initially, access will include the literature database and basic search functionality, but, as more validation is performed within our research group, more complex search functions and online visualization may be made available to the research community. With appropriate citation, we wish to promote the use of this database by interested academic parties. We also encourage users to upload their own reference data, making this an increasingly valuable online resource in functional ceramics research.

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REFERENCES AND NOTES

(1) Hewitt, R.; Gobbi, A.; Lee, M. L. A Searching and Reporting System for Relational Databases Using a Graph-Based Metadata Representation. *J. Chem. Inf. Model.* **2005**, *45*, 863−869.

(2) Borromei, R.; Cozzini, P.; Capacchi, S.; Cornia, M. Database of C-Glycosylporphyrins in Web Fashion. *J. Chem. Inf. Model.* **2000**, *40*, 1199−1202.

(3) Rose, S. Statistical design and application to combinatorial chemistry. *Drug Discovery Today* **2002**, *7*, 133−138.

(4) Woo, S.; Kim, K.; Cho, H.; Oh, K.; Jeon, M.; Tarte, N.; Kim, T.; Mahmood, A. Current Status of Combinatorial and High-Throughput Methods for Discovering New Materials and Catalysts. *QSAR Comb. Sci.* **2005**, *24*, 138−154.

(5) Bein, T. Efficient Assays for Combinatorial Methods for the Discovery of Catalysts. *Angew. Chem., Int. Ed.* **1999**, *38*, 323−326.

(6) Maier, W. F. Combinatorial Chemistry - Challenge and Chance for the Development of New Catalysts and Materials. *Angew. Chem., Int. Ed.* **1999**, *38*, 1216−1218.

(7) *NIST WebSCD: Structural Ceramics Database*. http://www.ceramics.nist.gov/srd/scd/scdquery.htm (accessed November 11, 2007).

(8) National Institute of Science and Technology. http://www.nist.gov/ (accessed November 11, 2007).

(9) *Dielectric Database Online*. http://www.ece.utah.edu/dielectric/ (accessed November 11, 2007).

(10) *MatWeb*. http://www.matweb.com/ (accessed November 11, 2007).

(11) Karditsas, P. J.; Lloyd, G.; Walters, M.; Peacock, A. The European Fusion Material properties database. *Fusion Eng. Des.* **2006**, *81*, 1225−1229.

(12) Coveney, P. V.; Fletcher, P.; Hughes, T. L. Using Artificial Neural Networks to Predict the Quality and Performance of Oil-Field Cements. *AI Mag.* **1996**, *17*, 41−53.

(13) Evans, J. R. G.; Edirisinghe, M. J.; Coveney, P. V.; Eames, J. Combinatorial searches of inorganic materials using the ink-jet printer: science, philosophy and technology. *J. Eur. Ceram. Soc.* **2001**, *21*, 2291−2299.

(14) *Functional OXide Discovery*; EPSRC Grant: GR/S85269/01. http://www.foxd.org (accessed November 11, 2007).

(15) McFarland, E. W.; Weinberg, W. H. Combinatorial approaches to materials discovery. *Trends Biotechnol.* **1999**, *17*, 107−115.

(16) Harvey, M. J.; Scott, D.; Coveney, P. V. An integrated instrument control and informatics system for combinatorial materials research. *J. Chem. Inf. Model.* **2005**, *46*, 1026−1033.

(17) Zhang, Y.; Chen, L.; Yang, S.; Evans, J. R. G. Control of particle segregation during drying of ceramic suspension droplets. *J. Eur. Ceram. Soc.* **2007**, *27*, 2229−2235.

(18) Pullar, R. C.; Zhang, Y.; Chen, L.; Yang, S.; Evans, J. R. G.; Alford, N. McN. Manufacture and measurement of combinatorial libraries of dielectric ceramics: Part I: Physical characterisation of $Ba_{1-x}Sr_xTiO_3$ libraries. *J. Eur. Ceram. Soc.* **2007**, *27*, 3861−3865.

(19) Pullar, R. C.; Zhang, Y.; Chen, L.; Yang, S.; Evans, J. R. G.; Petrov, P. K.; Salak, A. N.; Kiselev, D. A.; Kholkin, A. L.; Ferreira, V. M.; Alford, N. McN. Manufacture and measurement of combinatorial libraries of dielectric ceramics: Part II. Dielectric measurements of Ba1-xSrxTiO3 libraries. *J. Eur. Ceram. Soc.* **2007**, *27*, 4437−4443.

(20) Fearn, S.; Rossiny, J. C. H.; Kilner, J. A.; Zhang, Y.; Chen, L. High throughput screening of novel oxide conductors using SIMS. *Appl. Surf. Sci.* **2006**, *252*, 7159−7162.

(21) Frantzen, A.; Sanders, D.; Scheidtmann, J.; Simon, U.; Maier, W. A Flexible Database for Combinatorial and High-Throughput Materials Science. *QSAR Comb. Sci.* **2005**, *24*, 22−28.

(22) *OGSA-DAI*. http://www.ogsadai.org.uk/ (accessed November 11, 2007).

(23) *PostgreSQL*. http://www.postgresql.org/ (accessed November 11, 2007).

(24) *Digitize-Pro*. http://www.nuceng.com/Digitizepro.htm (accessed November 11, 2007).

(25) *Perl*. http://www.perl.com/ (accessed November 11, 2007).

(26) *PerlMol*. http://www.perlmol.org/ (accessed November 11, 2007).

(27) *Apache HTTPD project*. http://httpd.apache.org/ (accessed November 11, 2007).

(28) *PHP scripting language*. http://www.php.net/ (accessed November 11, 2007).

(29) Zhang, W.; Fasolka, M. J.; Karim, A.; Amis, E. J. An informatics infrastructure for combinatorial and high-throughput materials research built on open source code. *Meas. Sci. Technol.* **2005**, *16*, 261−269.

(30) Zhang, W.; Fasolka, M. J.; Karim, A.; Amis, W. J. An Open Source Informatics System for Combinatorial Materials Research. *Polym. Mater. Sci. Eng.* **2004**, *90*, 341.

(31) Fawley, W. J.; Piatetsky-Shapiro, G.; Matheus, C. J. Knowledge Discovery In Databases: An Overview. *AI Mag.* **1992**, *13*, 57−70.

(32) Scott, D. J.; Coveney, P. V.; Kilner, J. A.; Rossiny, J. C. H.; Alford, N. McN. Prediction of the functional properties of ceramic materials from composition using artificial neural networks. *J. Eur. Ceram. Soc.* **2007**, *27*, 4425−4435.

(33) Fielding, R. T.; Taylor, R. N. Principled design of the modern Web architecture. *ICSE '00: Proceedings of the 22nd International Conference on Software Engineering*, New York, U.S.A. 2000; pp 407−416.

(34) Cristianini, N.; Shawe-Taylor, J. *An Introduction to Support Vector Machines*; Cambridge University Press: 2000.

(35) Terfloth, L.; Gasteiger, J. Neural Networks and Genetic Algorithms in Drug Design. *Drug Discovery Today* **2001**, *6*, 102−108.
(36) Solmajer, T.; Zupan, J. Optimization Algorithms and Natural Computing in Drug Discovery. *Drug Discovery Today: Technologies* **2004**, *1*, 247−252.
(37) Lobanov, V. Using artificial neural networks to drive virtual screening of combinatorial libraries. *Drug Discovery Today: BIOSILICO* **2004**, *2*, 149−156.
(38) Rodemerck, U.; Baerns, M.; Holena, M.; Wolf, D. Application of a genetic algorithm and a neural network for the discovery and optimization of new solid catalytic materials. *Appl. Surf. Sci.* **2004**, *223*, 168−174.
(39) Landrum, G. A.; Penzotti, J. E.; Putta, S. Machine Learning models for Combinatorial Catalyst Discovery. *Meas. Sci. Technol.* **2005**, *16*, 270−277.
(40) Scott, D. J.; Manos, S.; Coveney, P. V. The Design of Electroceramic Compounds Using Artificial Neural Networks and Multi-objective Evolutionary Algorithms. *J. Chem. Inf. Model.* **2008**, *48*, 262−273.

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