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TOPICAL REVIEW — Physics research in materials genome

Discovery and design of lithium battery materials via high-throughput modeling*

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This paper reviews the rapid progress in the field of high-throughput modeling based on the Materials Genome Initiative, and its application in the discovery and design of lithium battery materials. It offers examples of screening, optimization and design of electrodes, electrolytes, coatings, additives, *etc.* and the possibility of introducing the machine learning method into material design. The application of the material genome method in the development of lithium battery materials provides the possibility to speed up the upgrading of new candidates in the discovery of lots of functional materials.

Keywords: Materials Genome Initiative, lithium battery materials, high-throughput simulations, material design

PACS: 88.30.gg, 82.47.Aa, 82.45.Gj, 82.45.Fk **DOI:** 10.1088/1674-1056/27/12/128801

1. Introduction

Recently, global warming caused by CO_2 emission is a serious issue in the world. The development of electric vehicles and renewable energy to reduce CO_2 emission is a priority task. Rechargeable batteries with higher energy density, longer cycle life and better safety are badly needed.[1] Lithium batteries are the key to the success of portable electronic products and electrical vehicles, and are the best choice for the energy storage devices of wind and solar power because of their high voltage, high specific energy density, rapid recharge capability and wide working temperature range.[2] The development of new materials is of major technological importance for lithium battery application. For example, the discovery of the layered-cathode $LiCoO_2$ and graphite anode realized the first lithium ion battery prototype;[3] the nano silicon-based anode has been demonstrated as an alternative with high reversible capacity of 380 mAh/g–2000 mAh/g;[4] the disclosure of $LiFePO_4$ provided the cathode with high thermal stability.[5] The indisputable fact is that the discovery of advanced materials and rational design play a key role in the field of lithium battery research. In the field of lithium batteries, the next goal is to develop all solid lithium secondary batteries.[6] By replacing the liquid combustible organic electrolytes traditionally used in lithium ion batteries, the inorganic solid electrolytes are expected to reduce the risks of leakage, vaporization and decomposition, and exhibit higher safety.[7,8] However, the lithium ion conductivity in solids is usually at least one order of magnitude lower than that in the liquid state, limiting the battery performance. Thus, the discovery and design of solid-state electrolytes with high ionic conductivity are of great importance to develop the next generation of lithium batteries. In addition, the requirement of high energy density is expected to be realized by finding electrodes with high voltage or high capacity.[9] Meanwhile, the solid–solid interface constituted by the electrode and the electrolyte in the solid-state battery needs to be designed with high thermodynamic, mechanical and electrochemical stabilities.[10]

To accelerate the pace of material discovery, a strategy named high-throughput (HT) combinatorial screening has been developed to search for new materials or to improve the properties of materials already in use.[11] The HT research method originates from the idea of the Material Genome Initiative and is promoted by the rapid progress of automation technology and computer technology in recent years. Different from the traditional method in which the creation, measurement and simulation of the samples are performed one by one, the HT methods synthesize and characterize new materials through thousands of samples in parallel, greatly speeding up the identification of valuable materials.[12] The HT techniques are also successfully applied in the discovery and design of new battery materials. Using a combinatorial and HT sputtering system, MacEachern *et al.* observed a new Fe–Zn alloy anode from thin film libraries of a Fe_xZn_{1-x} system;[13] by combining combinatory magnetron sputtering and HT structural determination, Borhani-Haghighi *et al.* identified compositions showing a layered structure in

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the $Li_a(Ni_xMn_yCo_z)O_r$ cathode library;[14] Beal *et al.* used an HT physical vapor deposition technique to optimize the ionic conductivity for solid-state electrolyte $Li_{3x}La_{2/3-x}TiO_3$ across a wide range of parameter space.[15] Simultaneously, the HT synthesis and measurement approaches, including the robot-type instruments producing large numbers of non-aqueous electrolyte mixtures,[16] the HT solid-state nuclear magnetic resonance probe for investigation of ionic conductivity[17] and the HT in situ pressure analysis for degradation processes[18] are also proposed for lithium battery studies.

The HT experimental investigation is showing great superiority in screening and optimizing within a specific composition space; nevertheless, the vastness of the combination of constituent elements and crystalline structures still challenges the discovery and design of the targeted materials in the unknown composition space. The HT simulation approach provides the opportunity to look through the wide range of structures and components for existing or virtual materials, and predict the intrinsic physical or chemical properties for each sample in advance. With the screening criteria determined by the application requirements, the candidates with the targeted performance can be selected and further optimized through HT experiments. The mutual promotion of HT simulations and experiments as shown in Fig. 1 is expected to accelerate the discovery of candidate compounds in the future and shorten the invested time and money not only for lithium batteries, but also for other new types of functional materials.[19] In addition, data mining and machine learning are introduced to benefit the understanding of the big data obtained from HT techniques, which provides chances to further explore the structure–property relationship of battery materials and understand the basic scientific questions regarding lithium batteries. This novel research method combining HT techniques, data science and artificial intelligence is known as the material genome approach and is expected to shorten the discovery and optimization process of new materials with high efficiency. This paper will present several HT simulation tools available for the discovery and design of new materials and provide examples of how candidate materials are uncovered for lithium batteries based on the material genome approach.

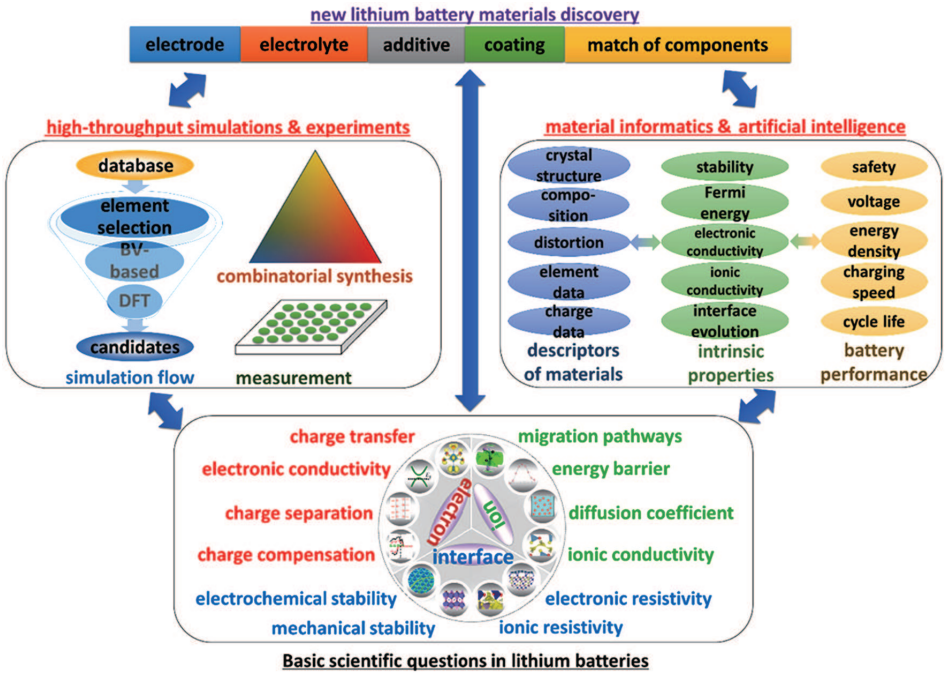


Fig. 1. (color online) The development mode of new material design in lithium batteries by means of HT techniques and data science.[19]

2. HT simulation tools for battery materials research

The key to realizing the HT simulations is to develop automatic computation flows which allow the tasks of structure selection, input generation, property simulation, output storage, data analysis and data expansion to be carried out automatically with minimal human intervention.[20] Several groups, as listed in Table 1, have established software to perform the automatic computational flows for HT simulations. The corresponding databases generated by these HT simulations are also provided. Some representatives include the Pymatgen and Fireworks packages[21,22] and the Materials Project,[23] the Automatic-Flow for Materials Discovery (AFLOW),[24,25] the Open Quantum Materials Database (OQMD),[26] the Automated Interactive Infrastructure and Database for Computational Science (AiiDA),[27] the Novel Materials Discovery (NOMAD) Laboratory,[28,29] the Computational Electronic Structure Database (CompES-X),[30] and the integrated HT computational platform MatCloud.[31]

Besides the frameworks created to perform the general processes of density functional theory (DFT) calculations, some programs designed for particular tasks also appear, *e.g.*, the material project-based python tool for the screening of interfacial systems (MPInterfaces),[32] the package for screening fast ion conductors based on the combination of simulation methods with difference accuracy (HT-iontrans)[33] and the database collecting the bond-valence-evaluated ion migration barriers for battery materials.[34]

Table 1. Several HT simulation tools and the established databases.

Developer	Toolkit	Database
Ceder group (USA)	Pymatgen, Fireworks[21,22]	Materials Project[23]
Curtarolo group (USA)	Automatic-FLOW[24]	Aflowlib.org[25]
Wolverton group (USA)	qmpy[26]	OQMD[26]
Marzari group (Switzerland)	AiiDA[27]	AiiDA
Scheffler group (Europe)	NOMAD[28]	NOMAD repository[29]
Xu group (Japan)	CompES	CompES-X[30]
Yang group (China)	MatCloud platform[31]	
Hennig group (Europe)	MPInterfaces[32]	
Chen group (China)	HT-iontrans[33]	Battery Materials DB[34]

The HT simulation tools mentioned above show some similarities. All the frameworks have the functions of preprocessing the structural models and input parameters, submitting and running the simulation tasks, data storage of the results and material candidate selection according to the data analysis. The screening criteria are varied according to the application requirements of the materials. For battery materials, the capacity, voltage, energy density, electronic and ionic conductivity and thermodynamic stability should be considered to select electrode materials.[35] For solid-state electrolytes, fast ion conduction is an important prerequisite. Meanwhile the electrochemical window, the chemical and mechanical stability between electrode and electrolyte, and electron insulation are also factors which must be considered.[36] Some properties, such as voltage and thermodynamic stability[37,38] can be relatively directly derived from the total energy calculations by HT-DFT. However, some properties, especially those related to the kinetic process, are difficult to simulate in the HT method. On one hand the computational cost is generally high for kinetic properties since the configuration or composition changes during the process; on the other hand the kinetic process is always complex and different among various structures making it hard to create a standard flow for all situations. One of the typical cases is the simulation of the ion diffusion properties. The most critical step in lithium batteries is the transport of lithium ions which intimately relates to the battery performance. The HT simulation tools on diffusion properties are only developed for face-centered cubic and hexagonal close-packed structures[39] and in the dilute vacancy mechanism.[40] To discover new solid-state electrolytes for next-generation lithium batteries, two kinds of ideas are proposed to solve this problem in different directions. One is to establish a holistic screening approach using high structural and chemical stability, low electronic conductivity and low cost to eliminate more than 90% of candidate materials, then a data-driven ionic conductivity model is adopted to classify the candidates into those with high and low likelihood of being superionic conductors based on existing experimental measurements[41] The screening flow is designed to use more constraints to cut down the number of candidates and avoid direct simulation on diffusion properties, but the pre-elimination reduces a lot of metastable structures which may be applied in reality. The other idea insists on evaluating targeted properties as screening criteria, but using the combination of calculation methods in different accuracy and screen step by step from low to high calculation accuracy.[42] Specifically, the fast bond-valence technique with lower precision is adopted for HT pre-screening and is able to provide the trend in the ability of ion motion in a wide range of compounds, then the time-consuming but accurate DFT method is used to do more precise transition state simulations only for those promising candidates assigned in the pre-screening process. Based on the idea of the combination of different precision calculation methods in the HT method, several new solid-state materials have been discovered.[42,43] All the HT simulation tools discussed here show great potential in the discovery and design of new lithium battery materials, and in the next section examples of the application of the above methods will be presented.

3. Application of HT modeling for the discovery of lithium battery materials

The fundamental material types applied in lithium batteries include the electrode, the electrolyte, the additive, the coating, *etc*. Each of them plays a distinctive role in the battery system and thus needs to meet different property requirements. We will describe a few examples in the following to show how

the HT modeling methods are of benefit to the discovery and design of various types of battery materials.

3.1. Electrodes

The exploration of new electrodes aims to find positive or negative electrodes with suitable operation voltages, capacity, and high thermodynamic and electrochemical stabilities to increase the energy density and safety of lithium batteries. Li-rich cathodes, composed of Li_2MnO_3–$LiMO_2$ (M = Mn/Ni/Co) compounds, yield a capacity exceeding 220 mAh/g but fast fading of the cell voltage during the cycling because of the transition metal migration and oxygen loss caused by the anionic redox processes.[44,45] Kim *et al.* performed HT-DFT simulations to optimize single- and mixed-metal Li_2MO_3 and $Li_2M_IO_3$–$Li_2M_{II}O_3$ compounds in Li-rich cathodes.[46] The screening is carried out according to the formation energy, thermodynamic stability, cell voltage, oxygen vacancy formation energy, metal migration tendency and mixing energy of the active/stabilizer element pair M_I–M_{II}. The top 30M_I–M_{II} active/stabilizer pairs are identified by the HT design strategy as shown in Fig. 2, and some new cathodes, such as Li_4IrSnO_6, are disclosed.[46]

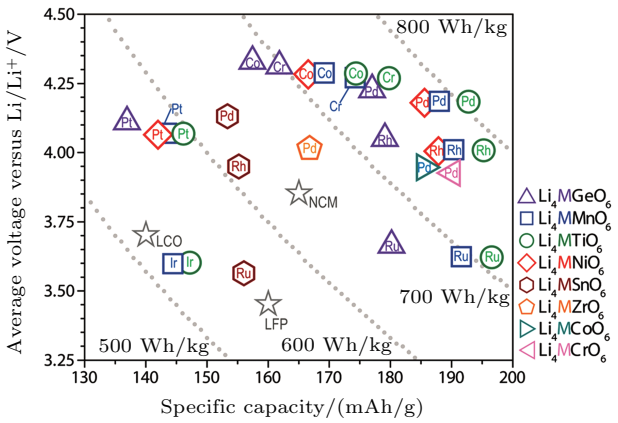


Fig. 2. (color online) Voltage versus capacity chart of the top 30 cathode pair candidates, ranked by gravimetric energy density among all calculated active/inactive $Li_2M_IO_3$–$Li_2M_{II}O_3$ cathode pairs.[46]

Besides the high energy density, a mechanical stable interface between the electrode and the solid-state electrolyte is also required in batteries since it is closely related to the cyclability and safety. To stabilize the solid/solid interface, the volume change of the electrode during lithium intercalation and deintercalation should be small enough. The electrodes showing negligible volume change are called low-strain electrodes. Nishijima *et al.* and Hajiyani *et al.* carried out HT-DFT screening of binary solid solutions in $LiFePO_4$ cathodes.[47,48] As shown in Fig. 3, through screening the effects of the doping pair on volume change during intercalation, the intercalation voltage, the energy density and the thermal stability with respect to the reaction with oxygen, the candidate solutions with low-strain properties are selected for the olivine phosphates.

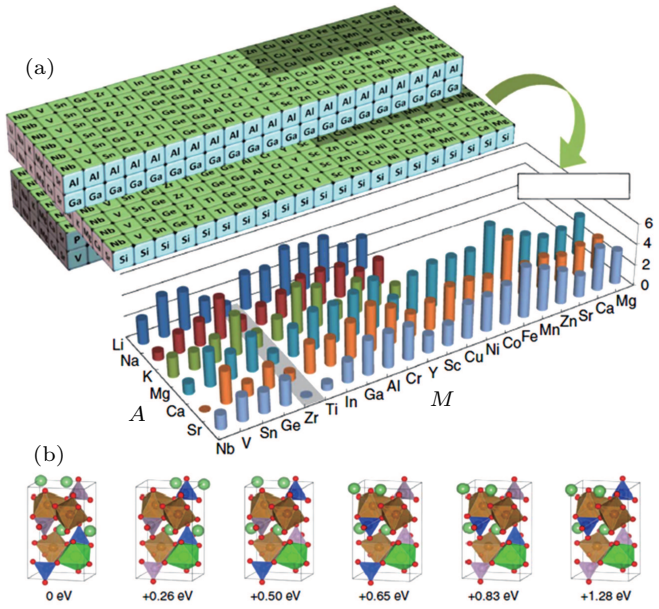


Fig. 3. (color online) Theoretical results of co-substituted $LiFePO_4$.[47]

The screening of anode materials is mainly carried out in alloy systems based on the conversion reaction mechanism. By screening the computational database based on gravimetric capacity, volumetric capacity, cell potential and volume expansion, several anodes, including $CoSi_2$, TiP and $NiSi_2$ are discovered.[49] The organic electrode materials can also be screened by HT simulations. By correctly describing the van der Waals interaction between organic molecules, the potentials of organic electrodes can be predicted successfully. Through highlighting the molecules with a relatively high potential, high capacity and small band gap, the targeted organic electrode candidates are proposed for experimenters.[50] Beyond the lithium batteries, the electrodes for some new energy conservation systems can also be screened by HT simulations, for example, the discovery of high-capacity electrodes for Li–O_2 cells[51] and spinel electrodes designed for Mg^{2+}, Ca^{2+}, Al^{3+} batteries.[52]

3.2. Solid-state electrolytes

Although investigations on fast lithium ion conductors have been widely performed, it is still not easy to grasp a comprehensive physical description for the ion migration phenomenon. To screen the materials with superior ionic conductivity, a scheme to combine the low-cost BV method and the highly precise DFT calculations provides a realistic strategy to screen solid-state electrolytes step by step.[42] One example is the optimization of lithium thiophosphate electrolytes, which have been regarded as promising candidates for solid electrolytes because of their improved ionic conductivities relative to their oxygen isologs.[53] However, the lithium-containing sulfides are usually more sensitive to moisture and are unstable in the air. HT simulations combing the BV and DFT methods have been performed to optimize the

β-Li_3PS_4 electrolyte by studying P-site doping and S-doping simultaneously.[42] The investigation process is illustrated in Fig. 4. According to the ion migration barriers obtained by the HT–BV calculations, the doping of O at the S position and the Zn–O co-doping schemes are selected as a promising way to improve both the ionic conductivity and the thermal stability in this system. Further DFT simulations with transition state theory reveal that the stronger P–O bond and the more space around it help to turn the 2D transport channels into 3D ones after doping as well as to activate the Li ions at 8d sites, which finally improve the comprehensive properties of the β-Li_3PS_4 system.[54] The experimental investigations have demonstrated the effects of O-doping and Zn–O co-doping on ionic conductivity and stability,[55] ensuring the success of the discovery and design of new electrolytes through HT modeling.

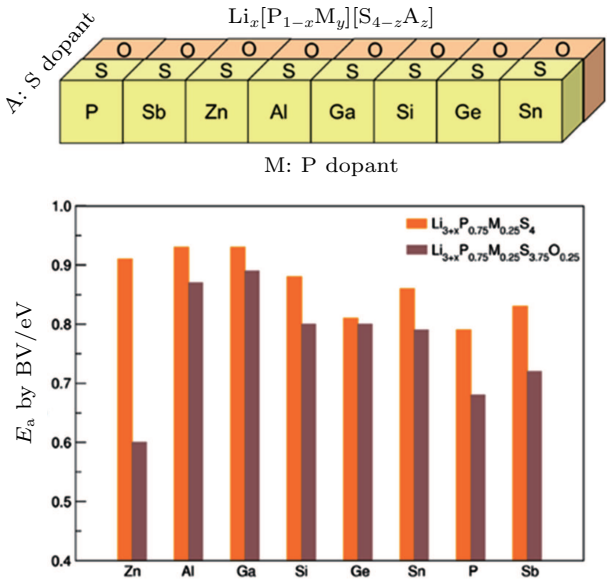


Fig. 4. (color online) (a) HT screening for the doping strategy of β-Li_3PS_4 by the combination of DFT and bond-valence calculations; (b) Calculated Li^+ migration energy barriers for Sb-, Zn-, Al-, Ga-, Si-, Ge-, Sn-doped P-site and O-doped S-site.[42]

The optimization doping scheme for the Li_3PS_4 electrolyte system by mixing O and S at the same atomic site stimulates researchers to look for new systems with mixed anions. As we know, although the sulfides show relatively higher ion conductivity, they are not easy to prepare and are unstable in the air, while the oxide electrolytes are easy to prepare and stable in the air, but their ionic conductivities are much lower. To integrate the advantages of sulfides and oxides, the HT crystal structure prediction is carried out in the configuration space of oxygen sulfides to explore new solid electrolytes.[43] A new solid-state electrolyte, LiAlSO, is predicted as shown in Fig. 5. It is in the structure of the *Pmc*21 space group and composed of AlS_2O_2 layers and Li ions between them. The transition state calculations based on the DFT method shows that the migration of lithium ions in LiAlSO is assisted by the coherent movement of the vacancy and interstitial ions with the energy barrier lower than 50 meV. Further simulations on the electronic structures ensure the wide electrochemical window in this system, ensuring that this compound can be a new promising solid electrolyte material.

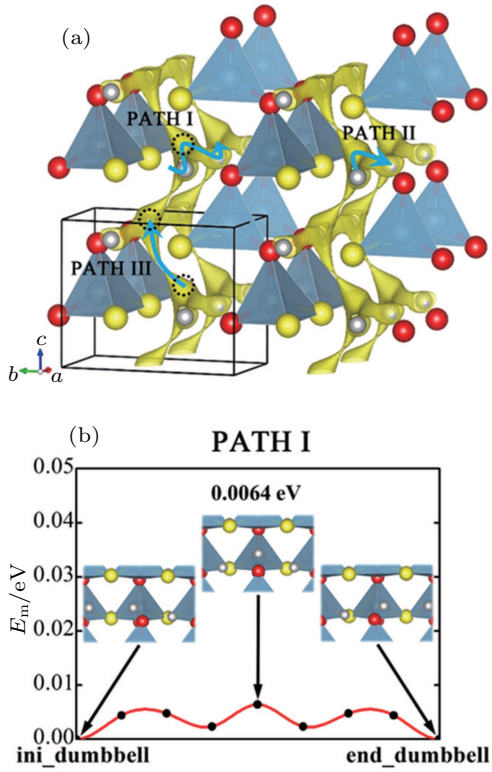


Fig. 5. (color online) (a) New oxysulfide LiAlSO designed by HT crystal structure prediction calculations; (b) the lithium ion migration barriers simulated using DFT method.[43]

Ion diffusion is a complex process and the simulation of migration barriers is time-consuming. However, data-driven machine learning models may help to discover the relationship between structures and properties, and aid in the discovery of new solid-state electrolytes. HT modeling and machine learning prediction are integrated in the study of LISICON-type electrolytes,[55] which greatly accelerate the design process in the huge compositional and structural phase space for the $Li_{8-c}A_aB_bO_4$ ($c = ma + nb$) system. Using HT first-principles molecular dynamics simulations, two superionic conductors, $Li_3Y(PS_4)_2$ and Li_5PS_4Cl, are predicted through the screening of the Li–P–S ternary and Li–M–P–S quaternary chemical spaces.[56] The traditional liquid electrolyte can also be designed or optimized in the HT modeling method. By performing large-scale virtual HT screening, candidate electrolyte solvents with high electrochemical stability have been discovered.[57–59]

3.3. Coating

In lithium batteries, the functional coatings on electrodes play an important role in suppressing the battery degradation. By preventing side-reactions and reducing transition metal

dissolution, it is hopeful that the proper selection of coating materials will prolong the cycle life of the batteries.[60] The HT simulation flow for coating materials is introduced in Ref. [60]. Besides the thermodynamic stability and the electrochemical stability, the properties connected with coating functionality, *e.g.*, physical barrier, HF barrier and HF scavenger, are also considered in the simulations. The material selection is a process with multi-objective optimization with weighted-sum and rank aggregation. By screening more than 1.3×10^5 oxygen-bearing materials, physical and hydrofluoric acid barrier coatings such as WO_3, $LiAl_5O_8$ and ZrP_2O_7, and hydrofluoric-acid scavengers, such as Sc_2O_3, Li_2CaGeO_4, $LiBO_2$, Li_3NbO_4, $Mg_3(BO_3)_2$, and Li_2MgSiO_4 are discovered.[60]

An attempt to select the coatings according to the lattice match between the electrode and electrolyte is also carried out. By screening more than 1000 kinds of lithium-containing compounds, the bond-valence calculated lithium ion migration barriers are sorted. The candidate ion conductors with crystal structures similar to the cathodes are selected as coating materials because they are expected to form a uniform stress interface much easier. For example, both Li_2SiO_3 and Li_2SnO_3 show similar layered structures to the Li-rich cathodes Li_2MnO_3, and the Li^+ migration pathways are also comparable as shown in Fig. 6.[61] Experiments have been conducted and confirmed the positive effects of Li_2SiO_3 and Li_2SnO_3 as coatings for Li_2MnO_3 to improve the cyclablity and capacity retention.[62]

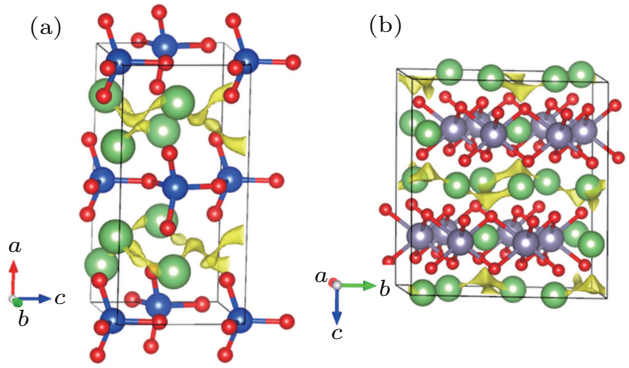


Fig. 6. (color online) The Li^+ migration pathways in (a) Li_2SiO_3 and (b) Li_2SnO_3 simulated by the bond-valence method.[62]

3.4. Additives

The screening of additives is mainly performed among organic molecules. Molecular properties like the highest occupied molecular orbital (HOMO), the lowest-unoccupied orbital (LUMO), the electron affinity and the chemical hardness are adopted as screening criteria.[63] Han *et al.* computed the HOMO and LUMO for 33 organic molecules and suggested five promising additives which are helpful in forming the solid electrolyte interphase.[64] Park *et al.* developed a search map for organic additive and solvent screening by combining a HT quantum chemical simulation with an artificial neural network algorithm.[65] Using the search map, the relationship between the redox potentials and functional groups is established as illustrated in Fig. 7.

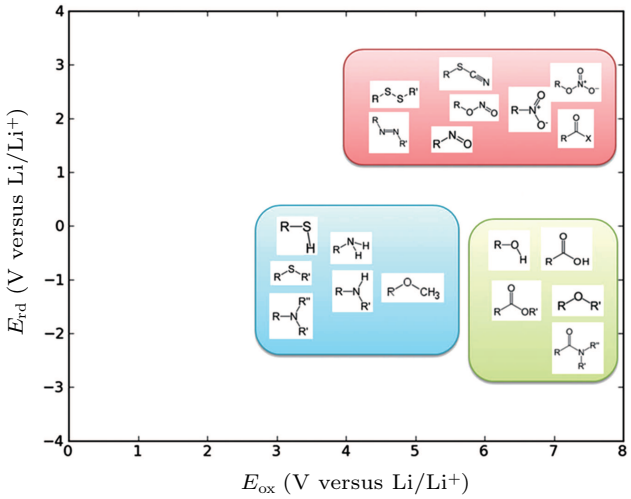


Fig. 7. (color online) Schematic diagram of the distribution of effective functional groups on the redox potential plane. Each functional group influencing redox potentials of organic molecules is positioned in the corresponding effective range of oxidation and reduction potentials.[65]

3.5. Safety of batteries

Thermal safety and high voltage are both important factors during battery design. The high energy density and power require the usage of high-voltage cathodes. However, the desired high thermal safety is hard to achieve simultaneously.[66] Jain *et al.* used HT-DFT to evaluate the link between voltage and safety for over 1400 cathode materials. The thermodynamic O_2 release temperature is used to assess the safety of the cathode.

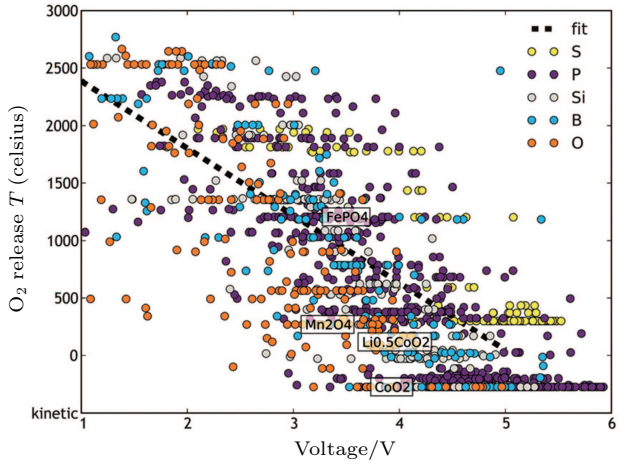


Fig. 8. (color online) Computed voltage versus computed decomposition temperature for 1409 cathodes investigated by HT computation.[66]

Figure 8 illustrates the voltage and safety data of different polyanion groups and redox couples. A few compounds

exhibiting both high voltage and high safety are screened out, providing opportunities for designing safe, high-voltage cathodes.[66]

4. Summary

The above examples of HT screening, optimization and design of electrodes, electrolytes, coatings, additives, *etc.* illustrate the feasibility of HT modeling in the development of new battery materials. To meet the material challenges in next-generation lithium batteries, advances in both science and technology are urgent in the materials genome research field. Designing automatic screening and predicting workflow with sufficient accuracy and efficiency is essential. For each part of the battery (the electrode, electrolyte, additive, collector, and so on) it is normal to meet more than one requirement to ensure the excellent performance of the whole device. Thus, screening and predicting tools for multiple objectives must be created. Besides the above, data science and technology is also an important research method in material design. It has been recognized that machine learning techniques and big data methods will play a more and more important role in solving the relationships between material properties and complex physical factors, which provides a tool to turn the data into knowledge and guide us in the material design, and vice versa. However, materials informatics is still an emerging field with difficulties like the lack of data standards, the diversity of material types, and even the conflict of research culture. In summary, rational design of lithium battery materials is highly desired in the near future. The advances in the development of HT techniques and material informatics bring a more efficient study mode and provide new opportunities to discover and design new battery materials, which also deepens our understanding of the basic scientific questions in battery fields and accelerates the discovery of materials for other new types of energy conservation device.

References

[1] Tarascon J M, Arm and M 2001 *Nature* **414** 359
[2] Goodenough J B and Kim Y 2010 *Chem. Mater.* **22** 587
[3] Novak P, Muller K, Santhanam K S V and Haas O 1997 *Chem. Rev.* **97** 272
[4] Li H, Huang X J, Chen L Q, Wu Z G and Liang Y 1999 *Electrochem. Solid-State Lett.* **2** 547
[5] Huang Y H and Goodenough J B 2008 *Chem. Mater.* **20** 7237
[6] Knauth P 2009 *Solid State Ionics* **180** 911
[7] Takada K 2013 *Acta Mater.* **61** 759
[8] Yao X, Huang B, Yin J, Peng G, Huang Z, Gao C, Liu D and Xu X 2016 *Chin. Phys. B* **25** 018802
[9] Shi S, Gao J, Liu Y, Zhao Y, Wu Q, Ju W, Ouyang C Y and Xiao R J 2016 *Chin. Phys. B* **25** 018212
[10] Yada C, Lee C E, Laughman D, Hannah L, Iba H and Hayden B E 2015 *J. Electrochem. Soc.* **162** A722
[11] Xiang X D, Sun X, Briceno G, Lou Y, Wang K A, Chang H, Wallace-Freedman W G, Chen S W and Schultz P G 1995 *Science* **268** 1738
[12] Curtarolo S, Hart G L W, Nardelli M B, Mingo N, Sanvito S and Levy O 2013 *Nat. Mater.* **12** 191
[13] MacEachern L, Dunlap R A and Obrov M N 2015 *J. Non-Cryst. Solids* **409** 183
[14] Borhani-Haghighi S, Kieschnick M, Motemani Y, Savan A, Rogalla D, Becker H W , Meijer J and Ludwig A 2013 *ACS Comb. Sci.* **15** 401
[15] Beal M S, Hayden B E, Gall T L, Lee C E, Lu X, Mirsaneh M, Mormiche C, Pasero D, Smith D C A, Weld A, Yada C and Yokoishi S 2011 *ACS Comb. Sci.* **13** 375
[16] Cartier C, Feng Z, Faulk J and Scherson D 2015 *ECS ElectroChem. Lett.* **4** A110
[17] Schiffmann J G, Kopp J, Geisler G, Kröninger J and Wüllen L 2013 *Solid State Nucl. Magn. Reson.* **49-50** 23
[18] Schiele A, Hatsukade T, Berkes B B, Hartmann P, Brezesinski T and Janek J 2017 *Anal. Chem.* **89** 8122
[19] Alberi K, Nardelli M B, Zakutayev A, *et al.* 2018 *J. Phys. D: Appl. Phys.* (in publication)
[20] Morgan D, Ceder G and Curtarolo S 2005 *Meas. Sci. Technol.* **16** 296
[21] Ong S P, Richards W D, Jain A, Hautier G, Kocher M, Cholia S, Gunter D, Chevrier V L, Persson K A and Ceder G 2013 *Comput. Mater. Sci.* **68** 314
[22] Jain A, Ping S, Chen W, Medasani B, Qu X, Kocher1 M, Brafman M, Petretto G, Rignanese G M , Hautier G, Gunter D and Persson K A 2015 *Concurrency Computat.: Pract. Exper.* **27** 5037
[23] Jain A, Ong S P, Hautier G, Chen W, Richards W D, Dacek S, Cholia S, Gunter D, Skinner D, Ceder G and Persson K A 2013 *Appl. Phys. Lett. Mater.* **1** 011002
[24] Curtarolo S, Setyawan W, Hart G L W, Jahnatek M, Chepulskii R V, Taylor R H, Wang S, Xue J, Yang K, Levy O, Mehl M J, Stokes H T, Demchenko D O and Morgan D 2012 *Comput. Mater. Sci.* **58** 218
[25] Curtarolo S, Setyawan W, Wang S, Xue J, Yang K, Taylor R H, Nelson L J, Hart G L W, Sanvito S, Buongiorno-Nardelli M, Mingo N and Levy O 2012 *Comput. Mater. Sci.* **58** 227
[26] Saal J E, Kirklin S, Aykol M, Meredig B and Wolverton C 2013 *J. Minerals Met. & Mater. Soc.* **65** 1501
[27] Pizzi G, Cepellotti A, Sabatini R, Marzari N and Kozinsky B 2016 *Comput. Mater. Sci.* **111** 218
[28] Ghiringhelli L M, Carbogno C, Levchenko S, Mohamed F, Huhs G, Lüders M, Oliveira M and Scheffler M 2017 *Npj Comput. Mater.* **3** 46
[29] http: //nomad-repository.eu/
[30] http: //compes-x.nims.go.jp/index_en.html
[31] http: //matcloud.cnic.cn/index.html
[32] Mathew K, Singh A K, Gabriel J J, Choudhary K, Sinnott S B, Davydov A V, Tavazza F and Hennig R G 2016 *Comput. Mater. Sci.* **122** 183
[33] Xiao R J, Li H and Chen L Q 2015 *J. Materiomics* **1** 325
[34] http://e01.iphy.ac.cn/www2
[35] Chen H, Hautier G, Jain A, Moore C, Kang B, Doe R, Wu L, Zhu Y, Tang Y and Ceder G 2012 *Chem. Mater.* **24** 2009
[36] Gao J, Chu G, He M, Zhang S, Xiao R J, Li H and Chen L Q 2014 *Sci. Chin. Phys. Mech. & Astro.* **57** 1526
[37] Ling S G, Gao J, Xiao R J and Chen L Q 2016 *Chin. Phys. B* **25** 018208
[38] Hautier G 2016 *AIP Conf. Proc.* **1765** 020009
[39] Angsten T, Mayeshiba T, Wu H and Morgan D 2014 *New J. Phys.* **16** 015018
[40] Wu H, Mayeshiba T and Morgan D 2016 *Sci. Data* **3** 160054
[41] Sendek A D, Yang Q, Cubuk E D, Duerloo K A N, Cui Y and Reed E J 2017 *Energy Environ. Sci.* **10** 306
[42] Xiao R J, Li H and Chen L Q 2015 *Sci. Rep.* **5** 14227
[43] Wang X L, Xiao R J, Li H and Chen L Q 2017 *Phys. Rev. Lett.* **118** 195901
[44] Xiao R J, Li H and Chen L Q 2012 *Chem. Mater.* **24** 4242
[45] McCalla E, Abakumov A M, Saubanère M, Foix D, Berg E J, Rousse G, Doublet M L, Gonbeau D, Novák P, Tendeloo G V, Dominko R and Tarascon J M 2015 *Science* **350** 1516
[46] Kim S, Aykol M, Hegde V I, Lu Z, Kirklin S, Croy J R, Thackeray M M and Wolverton C 2017 *Ene. Environ. Sci.* **10** 2201
[47] Nishijima M, Ootani T, Kamimura Y, Sueki T, Esaki S, Murai S, Fujita K, Tanaka K, Ohira K, Koyama Y and Tanaka I 2014 *Nat. Commun.* **5** 4553
[48] Hajiyani H R, Preiss U, Drautz R and Hammerschmidt T 2013 *Modell. Simul. Mater. Sci. Eng.* **21** 074004
[49] Kirklin S, Meredig B and Wolverton C 2013 *Adv. Energy Mater.* **3** 252
[50] Sun S, Chen Y and Yu J 2015 *J. Phys. Chem. C* **119** 25770

[51] Kirklin S, Chan M K Y, Trahey L, Thackerayc M M and Wolverton C 2014 *Phys. Chem. Chem. Phys.* **16** 22073

[52] Liu M, Rong Z, Malik R, Canepa P, Jain A, Ceder G and Persson K A 2015 *Energy Environ. Sci.* **8** 964

[53] Kamaya N, Homma K, Yamakawa Y, Hirayama M, Kanno R, Yonemura M, Kamiyama T, Kato Y, Hama S, Kawamoto K and Mitsui A 2011 *Nat. Mater.* **10** 682

[54] Wang X L, Xiao R J, Li H and Chen L Q 2016 *Phys. Chem. Chem. Phys.* **18** 21269

[55] Fujimura K, Seko A, Koyama Y, Kuwabara A, Kishida I, Shitara K, Fisher C A J, Moriwake H and Tanaka I 2013 *Adv. Energy Mater.* **3** 980

[56] Zhu Z, Chu I H and Ong S P 2017 *Chem. Mater.* **29** 2474

[57] Qu X, Jain A, Rajput N N, Cheng L, Zhang Y, Ong S P, Brafman M, Maginn E, Curtiss L and Persson K A 2015 *Comput. Mater. Sci.* **103** 56

[58] Borodin O, Olguin M, Spear C E, Leiter K W and Knap J 2015 *Nanotechnology* **26** 354003

[59] Korth M 2014 *Phys. Chem. Chem. Phys.* **16** 7919

[60] Aykol M, Kim S, Hegde V I, Snydacker D, Lu Z, Hao S, Kirklin S, Morgan D and Wolverton C 2016 *Nat. Communi.* **7** 13779

[61] Xiao R J, Li H and Chen L Q 2018 *Acta Phys. Sin.* **67** 128801 (in Chinese)

[62] Wang D D, Zhang X P, Xiao R J, Lu X, Li Y P, Xu T H, Pan D, Hu Y S and Bai Y 2018 *ElectroChim. Acta* **265** 244

[63] Halls M D and Tasaki K 2010 *J. Power Sources* **195** 1472

[64] Han Y K , Lee K, Jung S C and Huh Y S 2014 *Comput. Theor. Chem.* **1031** 64

[65] Park M S, Park I, Kang Y S, Im D and Doob S G 2016 *Phys. Chem. Chem. Phys.* **18** 26807

[66] Jain A, Hautier G, Ong S P, Dacek S and Ceder G 2015 *Phys. Chem. Chem. Phys.* **17** 5942