The Supercomputer Simulation of Nanocomposite Components and Transport Processes in the Li-ion Power Sources of new types

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Abstract. As a result of a large amount of computational experiments on a number of supercomputer resources quantum-chemical and molecular dynamic modeling of various nanocomposite components of Li-ion power sources was performed. Various aspects of transport, structural and energy processes inside LPS during numerous cycles of charging and discharge were simulated. By tools of molecular dynamics estimated influence of various external conditions on structure of nanocomposites and characteristics of above-stated processes.

Keywords: computer simulation, silicon-carbon nanocomposites, solid electrolytes, Li-ion power sources, VASP applied package, quantum chemistry, molecular dynamic

1 Introduction

In this article the main results of works on the project “Computer simulation of absorption and transport properties of solid electrolytes and nanostructured electrodes based on carbon and silicon in Li-ion power sources” are summed up. The aim of this project is the supercomputer simulation of quantum-chemistry and molecular dynamics of new nanocomposite materials (based on silicon and carbon) and solid electrolytes with high ionic conductivity, as well as non-reactive electrode materials during operation of a current source. Also, transports, structural and energetic processes occurring in the modeled nanostructures and at the “interface” between them have been simulated.

Li-ion power sources (LPS) are currently the most promising and common types of power sources and batteries. LPS are based on the transport of Li-ions through a liquid or solid electrolyte from cathode to anode (and back when charging). The design of new types of LPS is needed to improve their efficiency parameters, such as energy capacity, number of charge-discharge cycles, resistance to external conditions (temperatures), safety of their production and utilization from an environmental point of view, and cost (prime cost of materials in main components).

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Here is a brief description of the operating principle of Li-ion power sources.

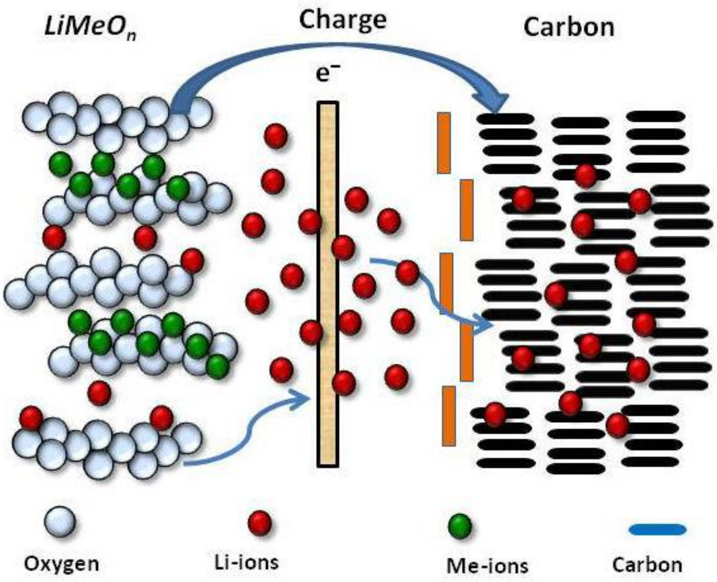


Fig. 1. Schematic diagram of a Li-ion power source

The following reactions occur in a Li-ion power source during charge:

on the positive plates:	on the negative plates:
$LiMeO_2 \rightarrow Li_{1-x}MeO_2 + xLi^+ + xe^-$	$C + xLi^+ + xe^- \rightarrow CLi_x$

The reverse reactions occur when discharging. Therefore, the modeling of lithiation processes (saturation of the anode by lithium == discharge process) and delithiation (lithium ions return to electrolyte and cathode == charging process) is basic for a comprehension of processes of functioning of LIA in general, estimation of the limiting factors and prediction of the most perspective nanocomposite materials.

Simulated materials should be the basis for the design and creation of new types of electrochemical and ecologically safe Li-ion power sources (LPS). These power sources will be able to operate at low and medium temperatures, provide significantly higher energy densities, and improve operational and cost characteristics.

The synthesis of new nanocomposite materials, the study of their properties and predictable applications are only possible as a result of a detailed computer modeling of crystalline composite structures, elementary processes and different mechanisms of chemical reactions and transport processes at molecular level.

Experimental studies of factors having a major influence on the solution of the issues listed above are complex, expensive, not always possible, and in most cases, do not give clear answers to the following questions: mechanisms of ongoing physical and chemical processes, reasons for their differences depending on the composition of the system and external conditions, possible directions of reactions, etc.

The experimental (analogue) simulation of the influence of various factors on the properties of the constituent components of Li-ion power sources and the processes occurring in them poses labor-intensive and costly tasks.

Since experiments give only initial and final information about processes, it is quite difficult to build a genuine analytical model. Such tasks can be solved partially in laboratory conditions, where analytic experiments give incomplete or indirect information about mechanisms and structures of experiment components. However, modern numerical methods of quantum-chemistry and molecular-dynamics simulation can provide substantial assistance in determining the characteristics of processes and assessing the impact of individual factors with a high degree of accuracy. These methods allow obtaining new theoretical data on the structure and properties of both nanostructured cathode-anode systems and ion-conducting solid electrolytes, making it possible to subsequently develop new highly effective materials for electrochemical devices.

A detailed simulation of elementary processes as well as mechanisms of lithiation/delithiation and ion-transport processes in Li-ion power sources at the micro level leads to a better control over chemical reactions occurring in them, allowing to design the most appropriate anode materials in terms of efficiency of electricity generation, lithiation processes, stability of materials during numerous charge-discharge cycles, cost of LPS constructive materials and environmental recycling processes.

Also, the created models can be reviewed for adequacy by comparing them (and the properties of materials modeled on their basis) against observable analytical, experimental and theoretical data published in specialized literature references.

For this task, the authors carried out a detailed quantum-chemical and molecular dynamic simulation of various nanosystems based on carbon and silicon, as well as solid electrolytes with high ionic conductivity, both in cluster approximation and for periodic boundary conditions with projector-augmented wave (PAW), using VASP, CPMD and Gaussian application packages on a number of high-performance computing resources [1-3].

The objects of the computer simulation are composites based on carbon and silicon, which have the ability to repeatedly absorb Li without damage and are promising materials for Li-ion power sources (nanoclusters, nanotubes, nanowires, nanopapers and active crystal surfaces). Also objects of this computer simulation are solid electrolytes with high ion conductivity based on glasses, salts and polymer composites that do not react with the electrode material during operation of a current source.

Some simulation experiments were conducted using authors’ computer system based on up-to-date software packages for quantum-chemistry and molecular dynamics, “hybrid” computing technologies, web services, data storage, visualization of results, etc. Using high-performance resources (supercomputers, problem-oriented clusters and hybrid systems) would greatly improve the details and the quality of the created models of nano-objects and those of the processes accompanying them, and would also allow to solve tasks previously inaccessible due to their computational complexity.

2 Simulation methods

The models of nanocomposite materials and processes occurring in them were constructed by methods of quantum chemistry computer simulation on the clusters of the Computation Center at the Institute of Problems of Chemical Physics (IPCP) and at the Supercomputer Center of Moscow State University "Lomonosov" [4], using the applied software packages VASP (Vienna Ab initio Simulation Package, https://www.vasp.at) and CPMD (Car-Parinello Molecular Dynamics, http://www.cpmd.org) for the calculation of complex nanostructures and the dynamics of their behavior depending on time and temperature.

The VASP applied package has been used by the authors during a long time for modeling materials and components of complex electrochemical objects. This package is applied to the simulation of various processes both in the volume and on the surface of solids (first of all, catalysis and ionic conductivity) within the non-empirical approaches based on the use of density functional theory with periodic boundary conditions and a plane wave basis set. VASP allows to optimize the structures and to model processes within a molecular dynamics framework.

VASP implements effective schemes of iterative matrix diagonalization and the highly efficient Broyden–Pulay electronic charge density mixing. In addition, the MSP processes convergence procedure (self-consistent field) and optimization are significantly improved, which greatly increases the efficiency of calculations. This package provides a good accuracy of description for structural and energy characteristics of systems containing up to several hundred atoms. First of all, we conducted a full optimization of the geometric and energy parameters of molecules under consideration within the established basis and method of calculation.

In this paper, we applied an approach based on density functional theory (DFT) with periodic boundary conditions to simulate learning systems. We applied the projector-augmented wave (PAW) with the corresponding PAW pseudopotentials and PBE functional (Perdew–Burke–Ernzerhof). The limit of energy (E_c) defining the completeness of the basis set was established at 400 eV. When simulating two-dimensional plates, the vacuum layer between them was not less than 10 Ǻ. To simulate the $Li_{10}GeP_2S_{12}$ electrolyte volume, we used a canned double cell $Li_{20}Ge_2P_4S_{24}$ involving 50 atoms; for the simulation of the surface, four such cells (200 atoms) were used.

To solve the problem of interaction of the surfaces between electrodes and electrolytes, we modeled (with full optimization of geometric parameters) a structure continuously propagating in two directions, solid electrolyte fragments (propagated $Li_{80}Ge_8P_{16}S_{96}$-fragment), a silicon-carbon paper (propagated $Si_{32}C_{38}$-fragment) and the result of their interaction (propagated $[Si_{32}C_{38}]*[Li_{80}Ge_8P_{16}S_{96}]$-fragment).

In the case of polymer electrolytes, we modeled (with full optimization of geometric parameters) the structure of infinite nanowires of Li*Nafion**nDMSO (n=0,1,8,16), and also spatially propagated fragments of $Li(C_{15}O_5F_{29}S)*n(H_6C_2OS)$ and $[Li(C_{15}O_5F_{29}S)*n(H_6C_2OS)]_2$ of 51 to 262 atoms.

For the optimization, we applied the Methfessel–Paxton method of electronic state (with blur parameter (σ) 0.2 and energy approximation of the value σ = 0). This approach allows for the automatic detection of system's multiplicity. The estimate of energy stability of combined systems was determined according to De/n(Li), computed as the difference between the calculated energy of the system and the total energy of isolated lithium atoms divided by the number of atoms of adsorbed lithium, for example, $De/n(Li) = -[E((SiC)_kSi_mLi_n) - E((SiC)_kSi_m) - nE(Li)]/n$.

We used two approaches for the simulation of transport processes in the framework of an ab initio non-empirical molecular dynamics with periodic boundary conditions: CPMD (Car-Parrinello approximation), in which the calculated wave function for the starting configuration is approximated by a set of classically-moving low-mass particles, and a more accurate but slower approximation, namely MD-VASP (MD/PBE/PAW), which uses the same algorithms as normal optimization structures, but with rougher calculation criteria.

Generally, the use of MD-VASP allows a substantially faster simulation than CPMD. MD-VASP requires about 6 to 8 times less computation steps to achieve the same penetration depth.

3 Computational complexity and efficiency of calculations

In earlier times, similar computer simulations were hindered by a catastrophic lack of computing resources, since calculating the behavior of small atomic clusters of the Si_{7-126} type, even in a simplified form, required months, and modeling systems as a whole (containing thousands of atoms) required approximately $n \cdot 10^6$ CPU-hours per year.

Only in recent times, the same simulation became feasible using high-performance supercomputing centers and grid polygons. Currently, the use of computing resources with speeds of the order of teraflops and petaflops allows to make sufficiently detailed simulations of geometrical and energy characteristics of modeled nanostructures. It is also possible to study the effects of various factors and processes occurring in these nanostructures for a variety of conditions determining the efficiency of the created LPS.

Let us summarize the computational complexity and use efficiency of computing resources in the process of quantum-chemical simulation of learnt structures. We used the IPCP cluster (15 teraflops: 176 dual-node HP Proliant, making a total of 1472 cores based on 4- and 6-core Intel Xeon processors 5450 and 5670 3 GHz, 8 and 12 GB of RAM per node; InfiniBand DDR communication network, transport and network management – Gigabit Ethernet; hard drives – no less than 36 GB per node), and the SCC of MSU supercomputing installations “Lomonosov-1,2” having various pools of processors (8 to 128 CPU) with obligatory presence of local drives and no less than 2 GB of RAM per core.

A sufficient effective acceleration of the VASP package for this type of tasks was observed for 40 to 48 CPU. The further growth of the efficiency of task parallelization is limited (or even reduced) by the rate of data exchange due to a significant increase in the amount of data being transferred between nodes. Thus, increasing the number of CPU over 48 (at least for this task variant) is meaningless for the moment. If the number of processors is more than 64, the dependence of the acceleration on the number of processors is practically absent or even falls [1].

The average effective time for calculation of Si_n clusters ($n = 2 \div 350$) and C_nSi_m nanofibers increases as the dimension of the silicon-carbon fragment increases, taking up to 4 days (78 hours on a pool based on 4-core Intel Xeon 5450 3 GHz processors) and even more (due to complications of the structure). The calculation time of lithiated large mesostructures of silicon and aggregates reinforced with nanotubes or nanowires took tens of days to complete.

The most critical calculation parameter is the amount of RAM per core, with an effect of acceleration of calculations with a decrease in the number of allocated cores by increasing the amount of RAM per core. For MD calculations, we used 14 000 steps per calculation (for example, heating up to 400 K for 2000 steps, holding at 400 K for 10 000 steps, cooling down to 10 K for 2000 steps, and optimizing the structure in standard mode; the time step model was 1 femtosecond). The calculation of complex structures, such as those described in Section 4.6, requires up to 80 000 CPU-hours.

In the latest versions of VASP, starting with version 5.4.1 (February 2015), the application package supports CUDA technology for the calculation method of standard and hybrid DFT (Hartree–Fock equation). For most tasks, using DFT on Tesla C2075 accelerators at the IPCP, we achieved (comparing VASP versions with support and without support of GPU acceleration on hybrid workstations with combination – 1 GPU with 2x6 cores CPU) 1.6- to 6-fold accelerations depending on the dimension of the problem and its type. This gives the prospect of a significant acceleration for VASP calculations on “hybrid” computing nodes (following VASP upgrade to versions above 5.4), including existing CPU-GPU pools on the SC “Lomonosov-1.2” and hybrid IPCP stations (in experiments we use combination 1 GPU Nvidia Tesla C2075 plus 2x6 CPU 3.46GHz Intel® Xeon® X5675, 48 Gb RAM). In addition to upgrading VASP, it is necessary to do a further reconfiguration of VASP settings files, and update CUDA library to version 7.5 (current version: 8.0).

The total number of computing experiments performed at all stages of the work reached more than 2000. If to speak about use of computing resources, then it is estimated as follows: SC "Lomonosov-1" (+"Chebyshev") – about 40-45% of experiments, IPCP cluster – 50%, IPCP and IEM workstations with GPU Nvidia support – 2-3%, MVS-100 – single experiments.

4 Simulation results

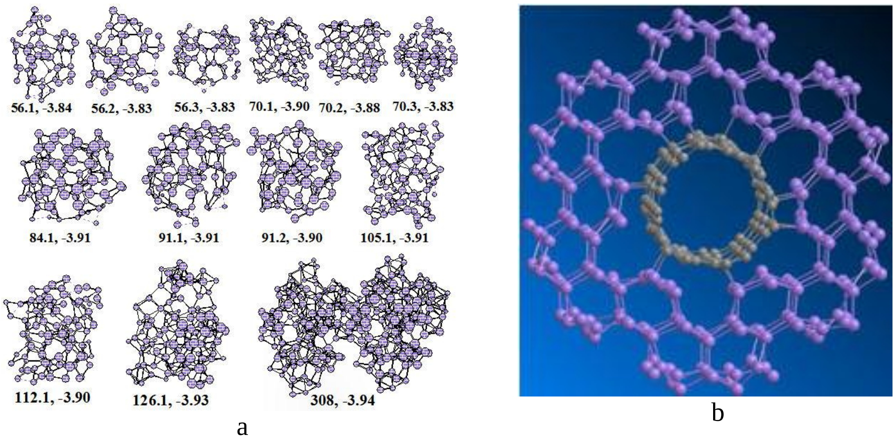
The results of the multi-step simulation have been described in detail in a number of publications by the authors of the present work [5-10]. Here is a brief description of the most representative results of the computer simulation of nanostructures and processes occurring in them.

4.1 Computer simulation of various types of porous nanocomposite materials based on carbon and silicon

Computer models of the following types of Si–C nanocomposites have been constructed by the authors [1, 5-6]:

1. pure silicon aggregates with different morphologies (clusters of “snowballs”, “core/shell”, etc., size up to 3 nm), and a number of silicon atoms ranging from 2 to 350;
2. silicon clusters with silicon carbide core (rod-shaped), 1.2 to 2.8 nm in diameter, and nanofibers of Si_nC_m type, n/m = 1÷3;
3. carbon nanotubes (CNT) with dimension (6,6) and 0.8 nm in diameter, surrounded by a layer of silicon clusters of various dimensions;
4. silicon nanowires with a rod on the basis of silicon carbide and silicon shell;
5. infinite carbon nanofibers coated with silicon nanoclusters;
6. silicon-carbon “nanopapers”.

A conclusion following from our research is that the use of different types of simulated nanocomposites may be a promising opportunity in the construction of new types of electrodes for LPS. Examples of the simulated nanostructures are shown in Figure 2.



a

b

Fig. 2. Examples of nanocomposites based on Si–C: a) mesoclusters Si_n (n = 56÷308); b) carbon nanotub with silicon atoms around Si_{288}/C_{120}. The models have been derived from the authors’ computer simulation using the VASP package (PBE/PAW level of calculation).

4.2 Quantum-chemical simulation of transport processes of lithium ions in nanocomposite materials based on carbon and silicon

On the basis of the constructed models of nanocomposites (see above), we made [7-9] a quantum-chemical simulation of various processes occurring during charge-discharge cycles of LPS (i.e. processes of lithiation and delithiation on electrodes based on the above-described nanostructures). A majority of characteristics of these processes have been established, including:

1. Li-ion transport processes and processes of lithium consistent implementation in Si–C nanostructures of various types and dimensions;
2. structural and energetic changes of nano-objects in processes of absorption of lithium atoms;
3. possible paths and migration barriers for lithium atoms in the process of nanoparticle saturation;
4. construction of models of sequential removal of lithium atoms from lithiated nanoparticles and determination of structural and energetic changes identified in this process;
5. determination of the limits of resistance to fracture for nanoparticles during delithiation processes.

4.3 Computer models of aggregation processes of initial and lithiated nanoparticles

In LPS operation, there are aggregation processes of small nanostructures into larger ones and vice versa, affecting greatly the characteristics of components and the whole LPS. We have obtained computer models of aggregation processes of original and lithiated nanoparticles [8, 9], including:

1. formation of a mesostructure based on original silicon-carbon nanoparticles;
2. formation of a mesostructure based on lithiated (saturated lithium atoms) silicon-carbon nanocomposite structures.

4.4 Quantum-chemical and molecular dynamics simulation of highly conductive solid electrolytes

This work presents the results of the computer quantum-chemistry and molecular dynamics simulation [10] of highly conductive solid electrolytes based on $Li_{10}GeP_2S_{12}$ systems and polymer electrolytes based on Li*Nafion*™ * dimethylsulfoxide (Li*Nafion* * 8DMSO) with an ionic conductivity that is higher than that of liquid electrolytes.

We modeled the structures and the contact surface of superionic solid electrolytes. In this connection, the ionic conductivity mechanism was determined during simulation. We also defined the types of surface structure and the nature of the $Li_{10}GeP_2S_{12}$ electrolyte contacts with anode nanocomposite materials (carbon fibers coated with Si_nC_m silicon nanoclusters and silicon-carbon “nanopaper”).

We modeled the contact surfaces of superionic solid electrolytes with different Si-C nanocomposites. It was shown that a layer of liquid or plastic polymer electrolyte, such as dimethylsulfoxide (hereinafter DMSO), can be used to enhance the contact between solid surfaces. The simulated structure and its surface are shown in Figure 3.

We constructed a computer model of interaction of solid and polymer lithium-based electrolytes with composites based on carbon fibers and silicon nanoclusters.

Lithium transition across the interface “electrode–electrolyte”, as well as the determination of the migration channels and the potential barrier were modeled taking as example the interaction of solid and polymer lithium electrolytes with composites based on carbon fibers and silicon nanoclusters.

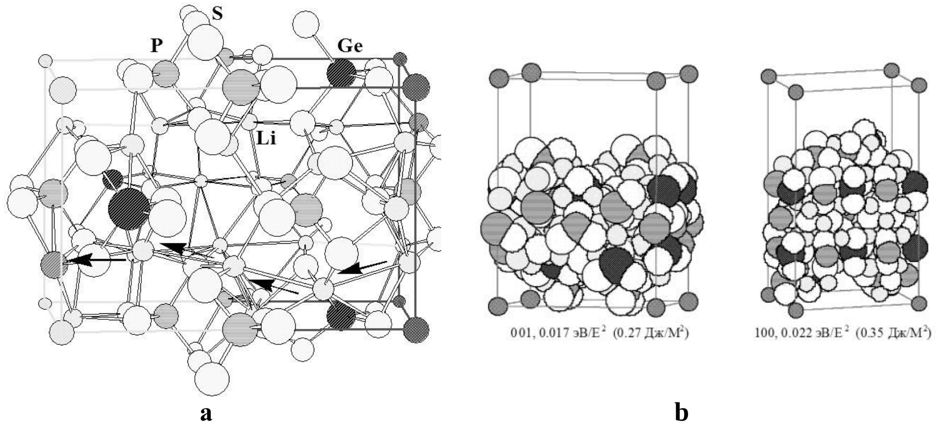


Fig. 3. Simulated structure (a) and (b) two types of modeled surfaces (001) and (100) $Li_{10}GeP_2S_{12}$ solid electrolyte crystal

4.5 Simulation of lithium ions migration in non-aqueous polymer electrolytes

Using methods of quantum chemistry and molecular dynamics, we modeled [2, 3, 10] various aspects of the migration of lithium ions in a complex electrolyte (Li*Nafion* * nDMSO, n = 0÷18) as well as the structure, stability and electronic properties of membranes based on the electrolyte, including the effect of various parameters, such as the degree of swelling of the electrolyte and a number of physico-chemical properties of the plasticizer containing the molar volume, the viscosity and the coordination number.

On the basis of the transport models, we made some conclusions on the possible paths of lithium migration and energy parameters: 1) four-coordinated lithium transition through three-coordinated state to the next position surrounded by four DMSO molecules, and 2) movement of the $Li(DMSO)^{4+}$ tetrasolvate complex.

4.6 Computer simulations of repeated lithiation/delithiation cycles depending on the degree of lithium saturation and temperature conditions

Along with the simulation of individual LPS components (electrodes, electrolytes) and processes occurring at the interfaces between them during operation of the battery, a great importance for the creation of new types of power sources is ascribed to the stability of these elements over time in case of multiple “charge-discharge” cycles, depending on the power capacity of the system (amount of lithium) and temperature conditions.

The molecular dynamics simulation is performed to assess the feasibility of the composite mesostructure return to its original state after repeated lithiation/delithiation cycles depending on the degree of lithium saturation and temperature conditions. MD-VASP (MD/PBE/PAW) approximation is used. For MD calculations, we used 14 000 steps per calculation (for example, heating up to 400 K for 2000 steps, holding at 400 K for 10 000 steps, cooling down to 10 K for 2000 steps, and optimizing the structure in standard mode; the time step model was 1 femtosecond). We took as initial model the nanocomposite models obtained in the first stages. The models are intended to illustrate the reorganization of the Li / Si layer structure during gradual recovery of lithium from the surface (i.e. discharge): the effect exerted by heating and subsequent cooling on the structure of silicon-carbon delithiated nanosystems and their possible return to the initial state according to the degree of heating of lithium and the saturation level.

The simulation has allowed to determine the most stable mesostructures for electrode materials, the optimal ratio of Li:Si in the Si–C nanocomposites saturation with lithium, and the best energy parameters of charge-discharge cycles. It has been demonstrated that the introduction of lithium into silicon is energetically more favorable than the formation of a metal layer on its surface, but increasing lithium concentrations leads to a reduction of energy difference, i.e. the implementation is less advantageous, the mesh of silicon atoms is broken into smaller pieces, the thickness of the absorbing layer is significantly increased, and its structure becomes amorphous. It is important to note that the energy in the modeled systems does not lead after cooling to stabilization to the substantial structural rearrangement that makes LPS components more resistant.

4.7 Computer model of ionic transport in lithium-ion batteries

We constructed computer models of ion transport using different combinations of the three main components of LPS, namely anode, cathode and membrane (electrolyte). These models allowed defining the basic characteristics of the energy system and evaluating the properties of the target battery based on calculations of the structure and transport properties of the electrode and electrolyte at molecular level. Comparing the results of different simulation options, we could identify the most promising areas of construction of lithium-ion batteries of new type and their characteristics during lithiation / delithiation.

Examples of the simulated complicate complexes “electrolyte–Si_nC_m” of different dimensions are shown in Figure 4.

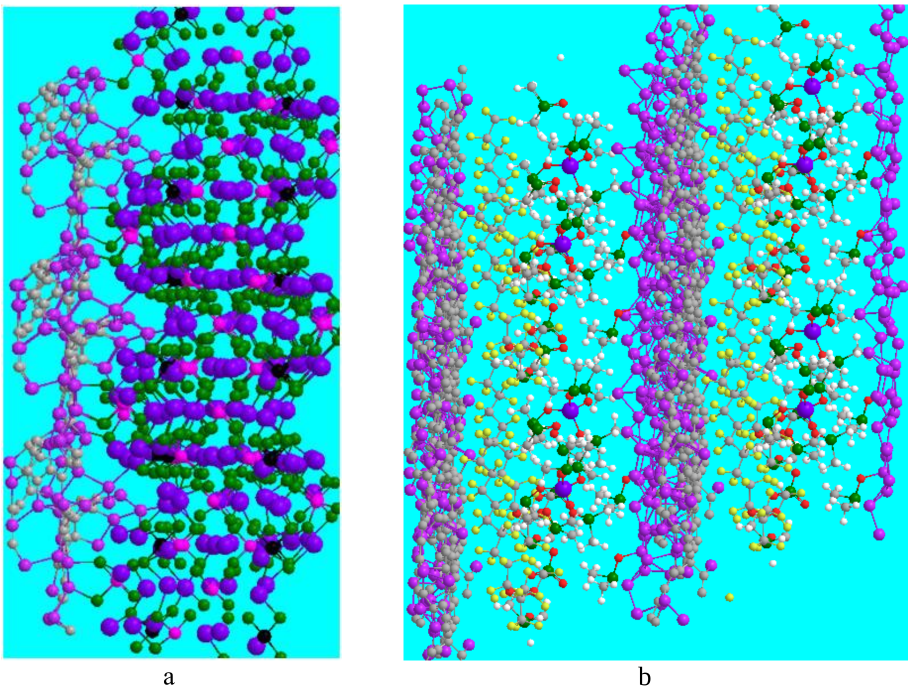


Fig. 4. Structure models of solid electrolyte complexes $Li_{80}Ge_8P_{16}S_{96}$ (a) and polymer electrolyte [LiNafion*8DMSO (b) with layers of $\mathbf{Si_{32}C_{38}}$ silicon-carbon "nanopaper"

4.8 Estimation of adequacy of created models

The assessment of adequacy, reliability and accuracy of the constructed computer models of nanocomposite materials and processes with their participation requires carrying out a number of tests of models by various methods.

In the model there should be no obvious contradictions to the observed physical and chemical effects in the evolution of real simulated systems (for example, during heating-cooling cycles) and the absence in the model of inconsistencies in the physical and chemical state of the simulated substances (for example, the formation of metallic lithium or the decomposition of electrolytes).

The program of tests of model includes the following methods:

1. comparison of the data obtained in the simulation with independent external data (analytical, experimental, theoretical, reference) by comparison of the received parameters, for example, the average bond energy of atoms in a crystal, the parameters of a crystal cell, photoelectronic absorption spectra, etc.) with earlier known from literature or reference sources;
2. comparison of simulation data of model operation received during the work of model in general to the data obtained earlier at model operation of separate components or processes with their participation;
3. check of a correctness and stability of work of model when using a wide range of

various combinations of the simulated substances – nanocomposite electrodes and solid/polymeric electrolytes at various external parameters and in the conditions of multiple cycles of a lithiation/delithiation;

4. assessment of a correctness and independence of work of model when carrying out computing experiments on various high-performance resources with different versions of the computer equipment (random access and disk memory, quantity of computed nodes, versions of the applied application packages)

The main test method is carrying out mass computing experiments on various computing resources on the basis of the created computer model with use of a wide range of input parameters with the subsequent analysis of the received results and selection of data for comparison. Further, the analysis of consistency of the received results from the point of view of physical and chemical criteria, correctness of the received results and their comparison to independent external data or to the array of previously obtained results of model operation which are carried out for separate components of model is carried out. For calculated quantitative parameters, a fairly accurate numerical estimate of the level of compliance with the directly observable data is possible.

It allows to estimate both the common adequacy of model to the simulated processes, and a correctness of use of the received results for analytical and expected conclusions regarding nanocomposite electrodes on the basis of carbon-silicon and solid/polymeric electrolytes for creation of new types of LPS.

The Gaussian software package (http://gaussian.com) was used for comparison and estimation of the accuracy of the simulation of some nano-objects at DFT/B3LYP level. By comparing different levels of calculation, we noted that the calculated values used in VASP and Gaussian software for average bond energies and distances of identical objects give consistent results with accuracy of 0.02 to 0.04 eV and 0.005 to 0.01 Å, respectively.

It should be noted that the difference of calculation results at B3LYP/6-31G (d, p), PBE/6-31G (d, p) and PBE/PAW levels does not exceed 0–2% for distances and 1–13% for energies. The chosen calculation level provides the following calculation accuracy in computer models: the Si crystal lattice calculated parameters a = b = c are 5.48 Ǻ (experimental: 5.43 Ǻ), the Si–Si distance is 2.37 Ǻ (experimental: 2.34 Ǻ), and the energy of the crystal is 4.44 eV (experimental: 4.52 eV).

The adequacy of the computer models was also evaluated by comparing the values calculated on the basis of their physical and chemical characteristics (optical and X-ray spectra, thermodynamic measurements, energy parameters) with those observed in physical experiments. For example, the calculated structural parameters for crystal electrolytes (a = b = 8.79 Å and c = 12.80) are in good agreement with X-ray experiments (a = b = 8.72 Å and c = 12.63 Å).

5 Conclusion

Thus, on the basis of a large number (more 2000) of numerical experiments regarding computer quantum chemistry and molecular dynamics simulation, we calculated the structures and surfaces of solid and polymeric electrolytes of a new type for LPS, their interaction with various nano-objects based on carbon and silicon with different morphologies, spatial rigidity, power characteristics, saturation potential with lithium ions. We also calculated transport processes of lithium ions (delithiation-lithiation) in nanocomposites, including structural energy characteristics and structures evolving over time (depending on the number of cycles of lithiation).

The model structures calculated, as well as the characteristics of electrolyte and anode materials for LPS and their interaction during charge and discharge were used to simulate a whole picture of lithiation and delithiation processes in Li-ion cells, the interaction of lithium ions with the surfaces of carbon and silicon nanomaterials, the determination of the “container” received by the anode materials, and also to model both components and new LPS types in general.

The simulation results will be used to determine the optimal conditions for the synthesis and production of the most energetically favorable and industrially suitable electrolyte and anode materials for new types of Li-ion power sources.

During the project are received the Certificate on the state registration of the database "Database on Structures and Physical and Chemical Properties Silicon and Silicon-Carbon Anodes for Lithium-Ion Accumulators" for No. 2016620100 and the Certificate on the state registration of the computer program No. 2017610081 "System of visualization of results of quantum and chemical modeling".

For the development of the "Database on the structures and physical and chemical properties of silicon and silicon-carbon anodes for lithium-ion batteries," received a diploma and a silver medal at the Moscow International Salon of Inventions and Innovative Technologies "Archimedes-2016".

For development "The database on structures and physical and chemical properties silicon and silicon-carbon anodes for lithium-ion accumulators" the author's team gained the diploma and a silver medal on the 19th Moscow International Salon of inventions and innovative technologies “Arkhimed-2016”.

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