Computational screening and descriptors for the ion mobility in energy storage materials

Mohsen Sotoudeh[1,*] and Axel Groß[1,2,†]

[1] *Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany*

[2] *Helmholtz Institute Ulm (HIU), Electrochemical Energy Storage, 89081 Ulm, Germany*

Abstract

Ion mobility in electrolytes and electrodes is a critical factor influencing the performance of batteries. Low ion mobility is for example one of the major factors reducing the range of battery-electric vehicles in winter time. On the other hand, with respect to the ion mobility in battery cathode materials there are scaling relations linking large insertion energies and thus high voltages with high migration barriers corresponding to low ion mobility. Consequently, a compromise has to be made between these two conflicting properties. In this opinion, we will address how computational screening and the identification of descriptors can accelerate the search for solid battery materials with improved ion migration properties, but we will also discuss how the scaling relations linking reaction and activation energies might be overcome.

Keywords: Batteries, ion mobility, electrodes, solid electrolytes, first-principles modelling

* mohsen.sotoudeh@uni-ulm.de

† axel.gross@uni-ulm.de

I. INTRODUCTION

Ion mobility is a critical performance parameter in batteries. Low ion mobilities lead to small charging and discharging rates and also dissipation losses which reduce both the power and the energy density of batteries. Hence there is a quest for battery materials with improved ion migration properties [1]. First of all it is important to note that there is a fundamental difference between the ion mobility in liquids and in solid materials. Whereas migration in liquids is in general a continuous process that can be driven by random processes or by gradients in some relevant property such as gradient or potential [2], migration in solids corresponds to hopping between local energy minimum sites [3].

In this opinion, we concentrate on migration in crystalline solids which occurs in batteries in the electrodes and in solid electrolytes. We will in particular review theoretical and numerical studies that address the ion migration in solids, discuss the basic methods to derive migration barriers, discuss descriptors for ion mobility, address scaling relations between reaction energies and migration barriers, and finally discuss workflows for computational screening studies to find materials with improved ion mobilities.

II. QUANTUM-CHEMICAL MODELLING OF ION MIGRATION IN SOLID BATTERY MATERIALS

From an atomistic point of view, ion migration in crystalline materials corresponds to the hopping of the charge carriers from one stable interstitial position to the next equivalent position hindered by an activation barrier. As the energetics play a crucial role in understanding these dynamics in battery materials, Density Functional Theory (DFT) calculations have become the method of choice for their reliable determination [4]. Still, in order to identify the position and height of the activation barrier, the energy minimum path between two equivalent sites needs to be identified, for example by transition state search routines [5]. The highest point along this path corresponds to the migration barrier. Together with the vibrational frequencies at the initial and the transition state, the kinetic rate constant for the hopping over the barrier can be derived using transition state theory [6]. Still, the determination of the energy minimum path is computationally rather demanding as it requires multiple evaluations of the energy of the migrating ion at several points between the initial and final state in a parallel fashion until the minimum energy path has been identified. Alternatively, activation barriers can be obtained through molecular dynamics (MD) simulations at different temperatures, assuming that the overall temperature dependence is determined solely by the Boltzmann factor. However, it is worth noting that these simulations are often even more numerically demanding.

To expedite calculations, two strategies have been introduced by Rong et al. [7]: the PathFinder algorithm, leveraging ion migration patterns, and the ApproxNEB, assessing image energy through cost-effective single-point DFT calculations. Combining these strategies provides an approximate prediction of E_a. An alternative approach is the bond valence site energy (BVSE) method [8], an empirical force field estimating energies around ionic sites.

Despite the success of DFT simulations in computational materials science, existing data may not fully meet the requirements for advancing the design of ionic conductors. These data bases predominantly emphasize information generated at zero temperature, overlooking anharmonicity and temperature-induced effects. Furthermore, current high-throughput and machine-learning studies focus predominantly on Li and Na, overlooking other cations such as Mg, Ca, K, and even neglecting anions such as O and halides. Achieving a comprehensive understanding of ion transport phenomena requires a balanced and thorough analysis of these diverse ionic classes that hold technological relevance.

III. DESCRIPTORS FOR ION MOBILITY

Descriptors reflect correlations between the materials properties and wanted or unwanted functions of these materials. The determination of descriptors can considerably speed up the search for novel materials with desired functional or multi-functional properties because once they are identified, only the particular descriptor needs to be optimized in the first step. One of the most famous examples of descriptors is the correlation between the oxygen binding energy of a metallic catalyst and its reactivity in terms of the oxygen reduction reaction [9], following the Sabatier principle. Descriptors have also been established in battery research. One example is the self-diffusion barrier of alkali and alkaline earth metals, which is correlated with the tendency of the corresponding metal anodes to exhibit dendrite growth [10]. With respect to the ion mobility in crystalline materials, there was the notion

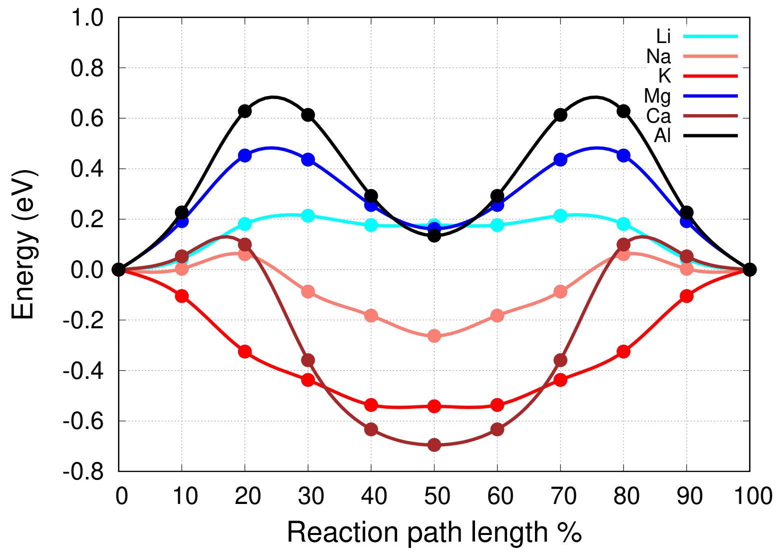

FIG. 1. Charge carrier migration in the ACr_2S_4 spinel structure with A = Li, Na, K, Mg, Ca, and Al. The energies are determined relative to the energy of the charge carrier in the tetrahedral coordination whereas the minima in the middle of the path correspond to the octahedral sites, using the set-up described in Ref. [12].

that still no common trends and mechanisms among different classes of ion conductors had been identified [1].

Typically, the size and charge of the migrating atom have been considered as determining factors as shown in Fig. 1 for spinel materials. For example, Na has the same charge as Li but is larger leading to a larger barrier with respect to the energy minimum position along a path from tetrahedral through octahedral to the next tetrahedral site. On the other hand, Mg has almost the same size as Li, but twice the charge, also causing a larger migration barrier. However, these two factors are not sufficient to capture a complete picture. The concepts of soft and hard ions have also been invoked, but not in a quantitative way [11]. Recently, these factors have been taken into account using the difference in electronegativity between the migrating cations and the counter anions of the host lattice [12]. As a descriptor for the height of migration barriers in crystalline materials, the so-called migration number was suggested:

$$N_{\rm migr}^{\rm AX} = (r_{\rm A} + r_{\rm X})\; n_{\rm A} n_{\rm X}\; \left(\chi_{\rm A} - \chi_{\rm X}\right)^2 \;\; . \tag{1}$$

Here, A corresponds to the migration ion, X to the counter ion of the host lattice, $r_{\rm A}$ and

n_X are their ionic radii, n_A and n_X the absolute values of the formal integer oxidation states, and χ_A and χ_X their electronegativities. By plotting calculated migration barriers as a function of this migration number, both for the variation of the migrating ion A and the counter ion X, linear scaling relations are observed [12]. This basically confirms the fact that in order to fully understand the migration mechanism, the deviation from a purely ionic interaction in a crystal structure must be taken into account [13]. Based on this descriptor and through computational analysis, a novel oxide spinel framework was characterized and predicted to exhibit high Mg conductivity [14].

Several additional features influencing ion mobility have been discussed in the literature, including lattice dynamics, phonon frequencies, and amplitudes [3, 15–17]. The polarizability of atoms, categorized as a chemical feature, has also been suggested as a potential correlate to ion migration [18, 19]. The crystalline lattice framework and structural features can play a role as well, with coordination geometries enhancing cation site stability and increasing migration barriers [20, 21]. Low energy barriers are observed in structures adopting a body-centered cubic (bcc) anion sublattice, facilitating direct hopping between tetrahedral sites [22]. Larger cell volumes, reducing migration barriers by enlarging the migration channel, are also influential [11], with larger, more polarizable anions contributing to this effect. Recently, a proposed structural feature promoting ionic conductivity involves corner-sharing connectivity in oxide crystal structures, attributed to distorted lithium environments and reduced interactions with non-lithium cations [23]. Through high-throughput computational screening, ten new oxide frameworks were discovered and experimentally validated in $LiGa(SeO_3)_2$, exhibiting notable ionic conductivity and activation energy of 0.17 eV [23].

Screening the spinel structures for different charge carriers revealed that the migration number served as a viable descriptor as illustrated in Fig. 2. However, for the lanthanide spinel compounds, the transition metal ionic radius was found to play a role in terms of stability and migration energy barriers [24]. The effect of lattice distortions due to atomic size mismatches is another important consideration, as it can reduce the barriers associated with certain ion migration pathways [25]. Furthermore, solids characterized by lower densities, such as high-temperature polymorphs and glasses, have demonstrated enhanced ionic conductivity due to 'paddlewheel' dynamics [26, 27]. Therefore, identifying a suitable descriptor is a daunting task due to the complex nature of migration reactions involving different diffusion mechanisms and pathways, highlighting the need for classification methods,

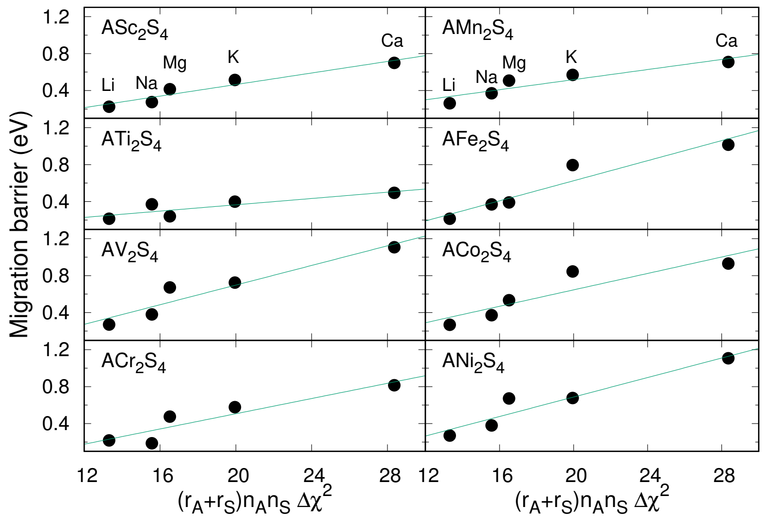

FIG. 2. Migration barriers obtained from DFT-NEB calculations versus migration number N_{migr} for AB_2S_4 spinel compounds with eight different transition metals B = Sc, Ti, V, Cr, Mn, Fe, Co, Ni and upon variation of migrating cations A = Mg, Na, K, Mg, Ca. Reprinted from Ref. [12], published under a CC BY license.

such as categorization based on mobile ions or lattice structures.

Machine learning (ML) provides a means to achieve these goals by identifying complex relationships between different features and a particular property. Recently Kim et al. [28] utilized ML to identify critical chemical and structural features that affect ion mobility in anti-perovskite lattice-based solid-state batteries, highlighting properties such as hopping distance and channel width. In another investigation, López et al. [29] utilized first-principles materials simulations and data analysis techniques to uncover that correlations between ion diffusivity and materials descriptors are most pronounced when linked to vibrational nature with anharmonic effects. Interestingly, elastic and vibrational descriptors, rather than conventional ones like chemical composition and ion mobility, prove to be more effective in categorizing solid-state electrolytes into universal groups. This highlights the significance of considering temperature effects in databases for an enhanced understanding and a generalized approach to energy material design. Optimizing these descriptors for ion mobility in energy storage materials is essential. A classification approach centered on the migration mechanism emerges as an appropriate strategy and by tailoring structural, electrochemical

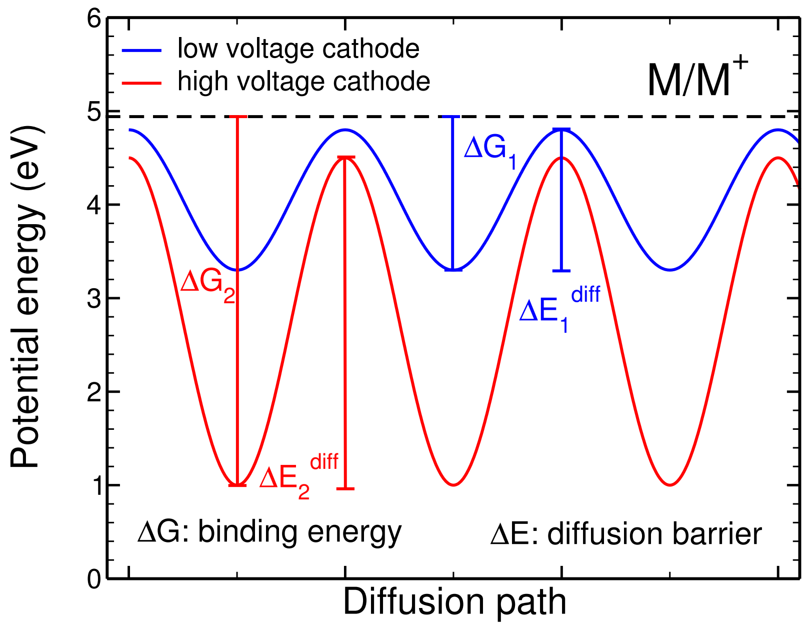

FIG. 3. Illustration of the scaling relations between binding energies and diffusion barriers in the migration in crystalline materials: The larger the binding energies, the higher the diffusion barriers for the propagation from one minimum to the next.

and transport properties, researchers can design materials with high ion mobility.

IV. SCALING RELATIONS IN CRYSTALLINE MATERIALS

In the previous section, we have concentrated on the ion mobility in crystalline materials, and identified factors that can lead to an high ion mobility. However, with respect to battery electrode materials, there are further important performance parameters, such as the energy density. In particular cathodes should exhibit robust charge carrier binding, as this directly impacts open-circuit voltage and, consequently, energy density [30]. Therefore, an ideal cathode should combine strong binding with low migration barriers for charge carriers.

However, in chemistry typically so-called Brønsted-Evans-Polanyi-type scaling relation [31, 32] between reaction and activation energies are observed. Such BEP relations also occur upon the insertion of atoms or ions into solid materials: The stronger the binding energies of the interstitials in the host materials, the larger the diffusion barriers hindering the migration from one binding site to the next. This is illustrated in Fig. 3. ΔG_1 is the relatively low binding energy of a metal atom in a host cathode material with respect to the cohesive energy of the metal. In order to increase the energy density of the corresponding battery, a stronger binding energy ΔG_2 is required. However, typically this is also associated with a higher diffusion barrier ΔE_2^{barr} hindering migration in this cathode.

Such BEP scaling relations have for example recently also been found with respect to the ion mobility in spinel materials [33]. As far as cathode materials in batteries of the rocking-chair type are concerned, large binding energies directly translate to high open-circuit voltages and thus to a high energy densities. However, according to these BEP relations, high energy densities and fast ion mobilities cannot be achieved for the same material. Hence a compromise between these two properties has to be made, as the combination of a high energy density and a facile ion migration requires to break these scaling relations.

However, there are examples of specific system in which scaling relation of the BEP type have been broken. For instance, single-atom alloy (SAA) catalysts allow to break the scaling relations between a high reactivity of a catalyst and strong binding of the reaction products. Such single-atom alloy catalysts typically consist of catalytically active elements atomically dispersed in an inert host metal [34], as for the H_2 dissociative adsorption on the PtCu SAA [35]. While the reactive Pt atom leads to a low barrier for hydrogen dissociation, whereas the resulting atomic hydrogen fragments only bind weakly to the Cu matrix.

The challenge is to transfer such a concept to the ion migration in crystalline solids. Typically the binding sites in solids correspond to highly coordinated configuration, for example six-fold coordination in octahedral sites or fourfold coordinated sites in tetrahedral sites, whereas the transition states have a lower coordination, for example a three-fold coordination in spinel materials [36]. Upon doping the spinel material by a very reactive atom, the effect of the dopant might be much stronger at the low coordinated transition state where often also the distances are much smaller than at the high-coordinated binding sites.

The effect of doping on the ion migration properties of solid electrolytes has been studied before [37, 38]. However, apparently non general conclusive trends could be derived so far. As doping is a statistical process and migration is associated with overcoming many barriers, the coordination effect described above might not be operative. Still overcoming the scaling relations between reaction energies and migration barriers can be so beneficial that we consider it worth the effort trying various approaches to break the scaling relations,

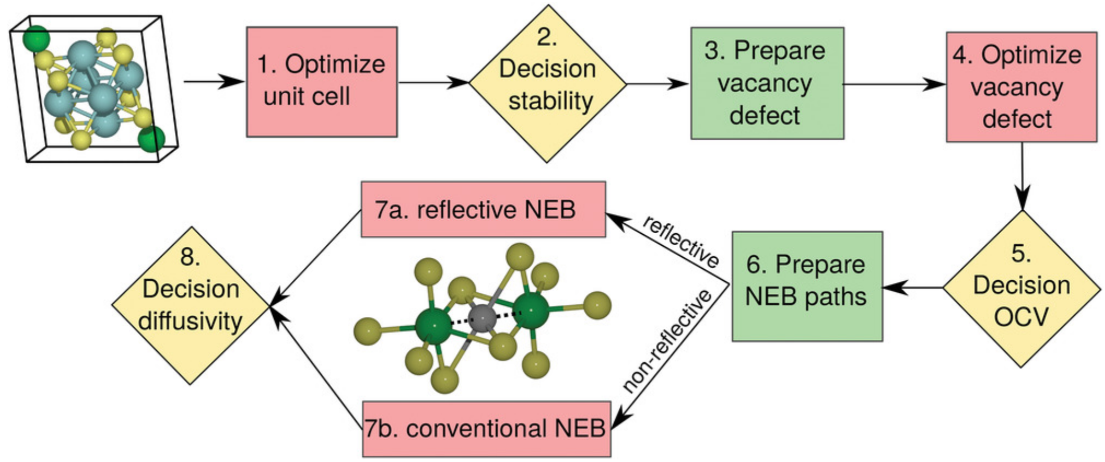

FIG. 4. Schematic representation of a workflow to accelerate the discovery of battery materials with improved migration properties. Reprinted from Ref. [42], published under a CC BY license.

V. COMPUTATIONAL SCREENING AND WORKFLOWS

Due to increase in computer power, computational screening techniques to accelerate the search for materials together with improved properties have become increasingly popular [39–41]. However, typically not only one materials property is of interest, instead there is an intricate interplay between different materials aspects. For example, all high performance materials are worthless if they are not stable under operating conditions. Therefore a structured approach is required to perform computational screening studies based on reasonable predefined workflows.

One such workflow to accelerate the discovery of battery materials with improved migration properties [42] is illustrated in Fig. 4. This workflow involves first an estimation of the stability of the candidate materials by calculating volume changes and the energy above hull. Open-circuit voltages are then derived by computing insertion energy in vacant site. Based on some predefined criteria it is then decided whether the computational expensive NEB calculations to determine migration barrier heights are performed.

This workflow has been used to find suitable cathode materials for Mg-ion batteries [43], considering ternary and quaternary structures taken from a database that contain Mg, oxygen and a transition metal. Thus two cathode materials are found that lead to a much higher open-circuit potential than the Chevrel phase which is considered to be the prototype cathode material for Mg-ion batteries [44]. Still, these high-voltage materials are also characterized by relatively large migration barriers above 1 eV, confirming the BEP scaling relations between reaction energies and migration barriers discussed above.

A similar workflow has also been used in a computational screening study restricted to perovskites materials, but taken the possible charge carriers Li, Na, K, Mg, Ca, Zn, and Al into account [45]. Thus in total 280 different perovskite compounds were tested. Determining first energy densities volume changes and the energy above, only 13 compounds survived as promising candidates for which the diffusion barriers were determined, resulting then in three remaining candidates that might be used in post-Li battery technologies with multivalent ions and which require further investigation.

VI. CONCLUSIONS

In this short Opinion, we have discussed computational and theoretical studies to find materials with improved ion mobility. Due to the increase in computer power and the development of powerful computational tools, numerical studies can nowadays have a significant impact in accelerating materials discovery. We have addressed the descriptor concept establishing correlations between materials properties and their corresponding ion mobility, showing promising examples which not only allow to identify suitable materials but also give a better understanding of the factors influencing ion mobility in crystalline materials. Still there are fundamental issues with so-called scaling relations between conflicting materials properties that might hinder optimizing several materials properties at once. Yet, there might still be concepts that allow to break these scaling relations. Finally, practical workflow schemes to perform effective computational screening studies have be addressed. Overall, the field of computational screening and descriptors for the ion mobility in energy storage materials is very active, and it can be anticipated that numerical approaches will significantly contribute to the accelerated discovery of materials with improved ion mobility properties.

VII. DECLARATION OF INTERESTS

none

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