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CalcOPP: a program for the calculation of one-particle potentials (OPPs)

Abstract: In recent years, one-particle potentials (OPPs) derived from neutron-diffraction data have become a popular means to estimate activation energies of ion migration in solids. Computer programs for their calculation, however, have mostly been private in-house solutions. The software *CalcOPP* presented herein permits calculating two- or three-dimensional OPPs either from probability density functions put out by the crystallographic suite *Jana2006/Jana2020* (including error maps) or from scattering-density maps reconstructed using the maximum entropy method (MEM) implementation *Dysnomia*. The title program is open-source, written in modern free-form Fortran and Python 3, and available free of charge under the permissive MIT License. Executables are published for 64-bit Microsoft Windows and Linux platforms and can be controlled via an intuitive graphical user interface or via command-line interface. Depending on the kind of input, *CalcOPP*'s output is readily visualized with standard crystallographic software or plotting applications. The release of the program not only makes the rather powerful OPP method more transparent, but it also opens it up to a broader, less programming-oriented public.

Keywords: activation energy; ion migration; maximum entropy method; neutron diffraction; probability density function.

1 Introduction

For a long time, solid-state scientists have been interested in mapping pathways of ion migration in crystalline solids and estimating the associated activation energies. But only recently, neutron diffraction at high temperatures has become one of the prime tools for such endeavors [1–8]. Data analysis in this quantitatively demanding and comparatively

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slow method (more specifically, structure solution) produces a spatial map of the scattering-length density (SLD) illustrating the positions and types of nuclei in the crystal. In the space- and time-averaging view of diffraction, fast motion of ions manifests as "smearing" of their associated SLD—much like in a long-exposure photograph of a moving object.

For the derivation of activation energies, ionic pathways are assumed to result from an effective potential that atoms experience while they are migrating (governed by attraction to and repulsion from the surrounding static framework). The approximation of each atom as an individual Einstein oscillator subject to Boltzmann statistics at the classical limit (potential energy much less than average thermal energy) gives rise to the one-particle potential (OPP) V [9]. For its calculation, two different approaches are employed: the PDF/OPP formalism, which relies on modelling the (joint) probability density function ([J]PDF), and the MEM/OPP formalism, which requires intermediate reconstruction of the SLD via the maximum entropy method (MEM).

1.1 The PDF/OPP formalism

To successfully use the PDF/OPP approach, one must model the Debye–Waller factors (DWFs) of the mobile ions adequately during structure refinement. Ellipsoids or even spheres that result from harmonic standard displacement models (often sloppily called "temperature ellipsoids") are only fit for the description of local vibrations. As the shapes of ion-migration pathways are generally rather complex and deviate from simple Gaussian distributions, DWFs for refinement have to be extended with anharmonic terms—usually via the mathematically convenient Gram–Charlier expansion.

The (J)PDF ("joint" indicating a superposition of several atomic PDFs) is the Fourier transform of the DWF(s) T_{anharm}. It signifies the probability $p(\boldsymbol{u})$ to find an atom displaced by a vector $\boldsymbol{u}$ from its reference position. Although the calculation of OPPs from PDFs is mathematically straightforward (cf. equation (1); k_B: Boltzmann constant, T: absolute temperature, $\mathbb{V}$: volume element under investigation), there are but few programs written for this purpose. The crystallographic computing systems *Jana2006/Jana2020* [10] (called *Jana*

hereinafter), e.g., can calculate PDFs from DWFs comprising anharmonic terms within three-dimensional (3D) cuboidal volume elements. However, they are only able to evaluate the resulting OPPs along coplanar polylines.

$$V(\boldsymbol{u}) = -k_B T \ln \frac{p(\boldsymbol{u})}{\max\limits_{\boldsymbol{u} \in \mathbb{V}} p(\boldsymbol{u})} \tag{1}$$

The PDF/OPP formalism is well-established and provides an inherent partition into densities associated with mobile ions and static framework. However, it is seldom used because of its requiring high data quality and completeness [1, 2].

1.2 The MEM/OPP formalism

The more recent MEM/OPP formalism, on the other hand, is less demanding and has thus become increasingly popular [3–8]. Therein, the OPP is calculated from the SLD ϱ_b in relation to a reference displacement (position) $\boldsymbol{u}_0$ according to equation (2).

$$V(\boldsymbol{u}) = -k_B T \ln \frac{\varrho_b(\boldsymbol{u})}{\varrho_b(\boldsymbol{u}_0)} \tag{2}$$

For this purpose, the solution of the phase problem is sufficient, an intermediate modelling step unnecessary. However, the SLD obtained via direct Fourier transformation of the refined structure factors contains artifacts that render it unsuitable—especially when dealing with powder diffraction data. As a remedy, the complex structure factors including their uncertainties are subjected to MEM reconstruction. In this iterative process, they are varied to achieve maximum variance within their uncertainty intervals under certain boundary conditions and criteria of convergence. The Fourier synthesis then results in a flattened SLD containing less artifacts. The crystallographic tools of choice for this method are programs like *Dysnomia* [11] (successor of *Prima* [12]) or *BayMEM* [13].

Unfortunately, MEM reconstruction does not yield SLD uncertainties, so OPP uncertainties are inaccessible. Because of the lack of a modelling step on this route, the SLD associated with a migration pathway may furthermore be "tainted" by adjacent vibrating ions: At any point in space, only a summary SLD without a-priori assignment to an atom is calculated.

The subsequent treatment of the SLD as a probability density (compare equations (1) and (2)) seems plausible but hitherto lacks strict mathematical foundation. For it to be sensible, the SLD must represent the mobile atoms under investigation adequately, i.e., describe their distribution

exclusively and completely.[1] Furthermore, a probability density function has to be non-negative, Lebesgue-integrable, and normalized to an integral of unity over the whole space. The following hand-waving rationale suggests that a ratio of SLDs within carefully chosen limits shares the properties of a probability density ratio:

– *Adequacy:* If the negative/positive scattering-length density is solely generated by the crystallographically unique atom under scrutiny, the former is an adequate measure for the distribution of the latter. In some other cases (another static negative/positive scatterer), it is adequate if the scope is limited to areas accessible to the atom under scrutiny only (i.e., the environment of its migration pathways).
– *Non-Negativity:* Only non-negative ratios (both SLD values either negative or positive) are considered.
– *Integrability:* Discretely sampled SLDs are Lebesgue-integrable.
– *Normalization:* For ratios of density values, normalization is unnecessary (the normalizing constant cancels).

Figure 1 gives an overview over the steps, tools, and data types within both formalisms. A more general introduction into the mapping of ion diffusion pathways and diffraction-based estimation of the associated activation barriers has already been published [14].

So far, only unpublished and undocumented programs (mostly, simple scripts) have been used to calculate OPPs from 2D/3D PDF and 3D SLD data. Herein, the program *CalcOPP 2.0* [15] is presented, which was designed according to the following criteria:

– simple installation,
– graphical user interface (GUI) with integrated documentation,
– source code written in contemporary languages and dialects,
– permissive free-software license, and
– public availability and citability.

2 Program specification

I had written the core of the two modules for calculating OPPs in Fortran before *CalcOPP* was conceived of. The GUI's source code and the module for the calculation of OPPs from scattering densities, on the other hand, were

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[1] This is the main reason why data from X-ray diffraction is of little use without extensive correction or deconvolution. The spatial distribution of electron density depends on the element and is deformed by chemical bonds, lone pairs, etc.
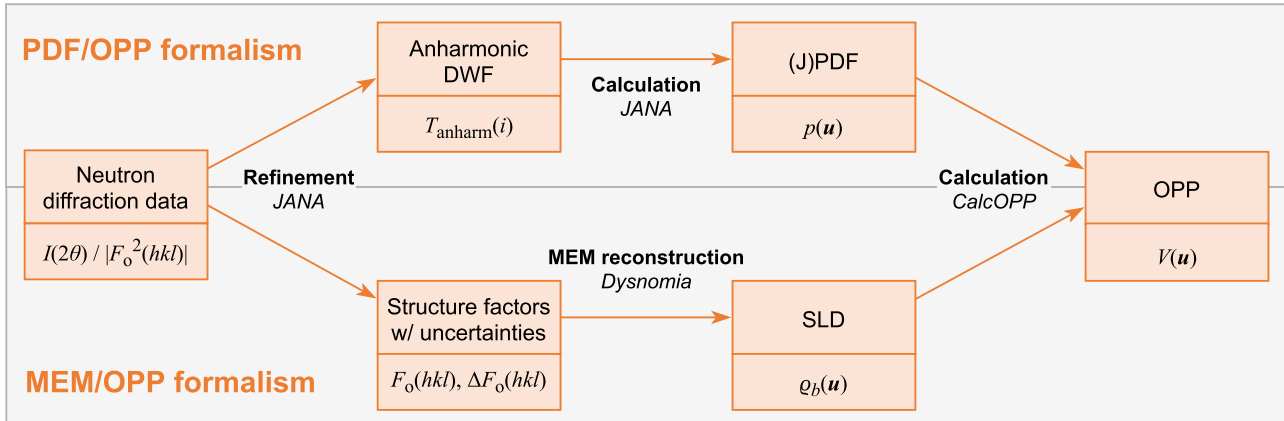
Figure 1: Procedure for calculating the OPP from neutron-diffraction data with intermediate steps and typical software tools. I: Diffraction intensity, 2θ: diffraction angle, F_o: observed structure factor, hkl: Bragg indices, i: index over crystallographically independent atoms.

advantageously written in Python. While Fortran programs are compiled into executables ahead-of-time, Python programs are interpreted just-in-time. The package *PyInstaller* [16] facilitates freezing/packaging them for distribution. Resulting program archives just have to be downloaded, unpacked, and locally executed. Compressed archives for the 64-bit versions of Microsoft Windows and Linux are available.

The source code is published under the MIT License (the Expat License, to be precise), which grants any person unrestricted dealings in the software—including use, copying, modification, merging, publishing, distribution, sublicensing, and/or sale of copies—if the license and the copyright notice (comprising the proof of authorship) are part of all copies or substantial portions.

The acceptance of new information technologies (and, thus, of new software tools) seems to be influenced more strongly by common beliefs than by individual differences in attitude [17]. At the same time, GUIs are widely considered easier to operate than command-line interfaces (CLIs) [18]. This conforms to the personal experience of an unwillingness to use the command line—even amongst scientists.[2] Without giving proof of a general superiority, studies indicate that beginners learn the use of GUIs more swiftly and more efficiently [19, 20]. As best practices recommend [21], *CalcOPP* comes with a CLI (making it also accessible for automated scripts) and a GUI. The effort of building the user interface was manageable employing the Python package *PySimpleGUI* [22] (see Figure 2, left panel). On the left side, the GUI shows a context-sensitive documentation, which provides general instructions and warnings as well as

information on prerequisites, input preparation, options, and handling of output data. The GUI's right side allows choosing data source and parameters. It also displays the text output of the program modules.

CalcOPP accepts input data sampled in 2D or 3D along a uniform grid. Its interface is designed to accept direct exports/temporary files created by *Jana* and native outputs of *Dysnomia* [11]. Depending on the kind of input data, the program works in three different modes (see Table 1). Computed 3D OPPs can be visualized without further conversion using the well-known tool *Vesta* [23].

2.1 Calculation of OPPs from 2D PDFs

Two features of this mode merit additional explanation. Firstly, it permits the reformatting of PDF input data, thus making them easily accessible for standard plotting applications (like *gnuplot, QtiPlot, Origin*, or *Igor Pro*).

Secondly, *CalcOPP* can estimate the OPP uncertainty based on a PDF error map calculated by *Jana* via its implemented Monte-Carlo method [24]. Unfortunately, several problems prohibit the use of standard models for the propagation of uncertainty:

– In regions of high probability density (e.g., near atom positions), strong correlation between local and maximum values occurs. This leads to an overestimation of the OPP uncertainty.
– In regions of low probability density (e.g., at bottleneck positions), the relative uncertainties may be too large to warrant treatment by expansion of a Taylor series—particularly when truncating after the linear term.
– The distribution of values depends on the problem under investigation. In general, it is neither normal nor log-normal.

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2 As this statement is based on a small sample from the author's social environment (working and training groups, conferences), it is to be regarded as strictly anecdotal.
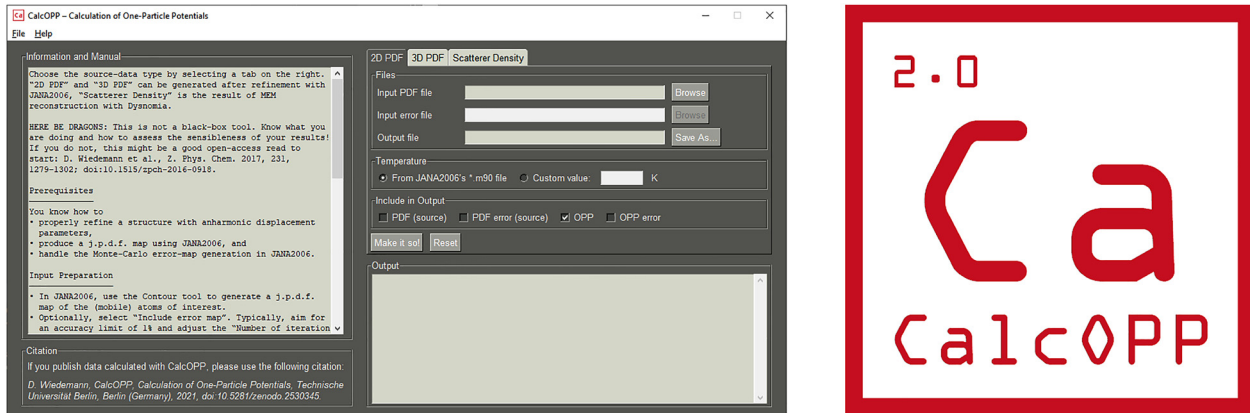
Figure 2: The program *CalcOPP 2.0*. Left: screenshot of the GUI of version 2.0.5 under Microsoft Windows 10. Right: project logo.

Table 1: Input and output data for the three modes of *CalcOPP 2.0*.

Input			Output	
Type	**Source**	**Source format**	**Target**	**Target format**
2D-PDF	JANA	Structured file (*.stf)	Plotting software	ASCII text (*.asc)[a]
3D-PDF	JANA	XCrySDen structure (*.xsf)	VESTA	*XCrySDen* structure (*.xsf), *VESTA* file (*.vesta)
3D-SLD[b]	Dysnomia	Periodic grid (*.pgrid)	VESTA	Periodic grid (*.pgrid), *VESTA* file (*.vesta)

[a]Handling of uncertainties (see section 2.1) as well as simultaneous or separate reformatting of PDF data possible. [b]Use of electron-density data, in principle, possible under application of extensive corrections (see section 1.2).

– The interval of PDF uncertainty is considered symmetrical with respect to its central value. Thus, the one of the (logarithmically dependent) OPP must be asymmetrical.

As *CalcOPP* cannot access the covariance of maximum and local probability densities, it is unable to solve the first problem. This limitation must be kept in mind when evaluating the OPP near its minima.[3] To circumvent the other issues, *CalcOPP 2.0* calculates the upper and lower limits $\Delta_\pm V(\boldsymbol{u})$ of the OPP uncertainty interval according to equation (3) instead of propagating uncertainties.

$$\Delta_\pm V(\boldsymbol{u}) = -k_{\mathrm{B}}T \ln \frac{1 \mp \left|\dfrac{\Delta p(\boldsymbol{u})}{p(\boldsymbol{u})}\right|}{1 \pm \left|\dfrac{\Delta p\left(\arg\max\limits_{\boldsymbol{u}\in\mathbb{V}} p(\boldsymbol{u})\right)}{p\left(\arg\max\limits_{\boldsymbol{u}\in\mathbb{V}} p(\boldsymbol{u})\right)}\right|} \quad (3)$$

2.2 Calculation of OPPs from 3D SLDs

The OPP is calculated from the scatterer density ϱ (usually, the SLD) according to equation (4). In contrast to PDF-based computation, it is not generally possible to use the global maximum as a reference position, because negative (e.g., lithium ions in neutron diffraction) or comparatively weaker scatterers (e.g., mobile silver besides static iodide ions in neutron diffraction) may be under scrutiny. That is why the user must set the reference density ϱ_0 to a global or local extremum according to the problem at hand. For this purpose, *CalcOPP* allows choosing the global minimum, the global maximum, or a manually determined local value ϱ_{loc}.

$$V(\boldsymbol{u}) = -k_{\mathrm{B}}T \ln \frac{\varrho(\boldsymbol{u})}{\varrho_0} \quad \text{where } \varrho_0 = \min_{\boldsymbol{u}\in\mathbb{V}} \varrho(\boldsymbol{u}) \quad \vee \quad \varrho_0$$

$$= \max_{\boldsymbol{u}\in\mathbb{V}} \varrho(\boldsymbol{u}) \quad \vee \quad \varrho_0 = \varrho_{\mathrm{loc}} \quad (4)$$

3 Examples

Several examples of the use of *CalcOPP* and its routines were published in peer-reviewed journals. Most of these deal with mapping lithium-ion migration pathways and estimating the associated energy barriers. This is the case for the lithium-deficient 2D conductor Li$_x$TiS$_2$ [25] and for
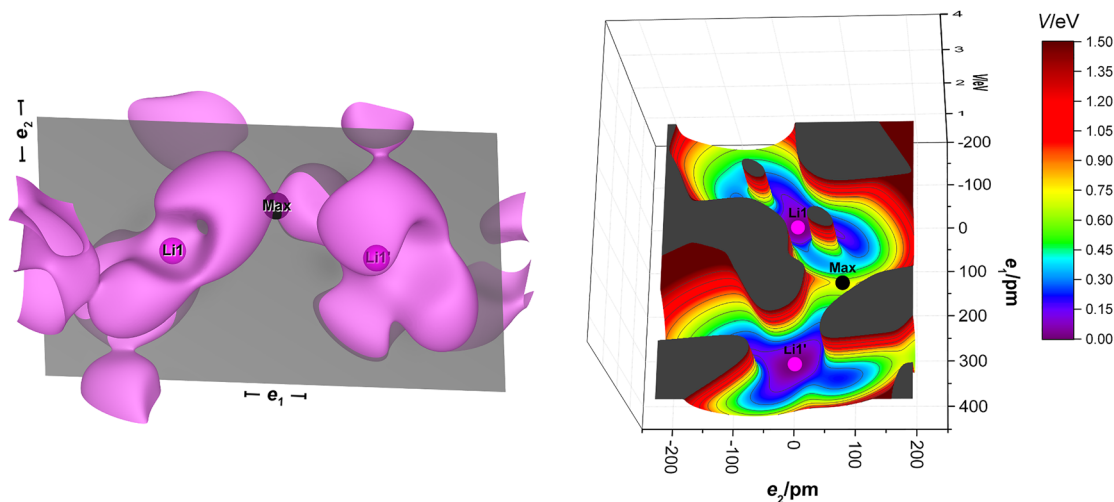
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3 To estimate activation barriers for ion migration, the OPP is evaluated at its local maxima. In these cases, this limitation should not be an issue.

Figure 3: Optimal diffusion path between two adjacent lithium positions (pink: Li1, Li1′) and position of the OPP maximum (black: Max) in γ-LiAlO$_2$ at 1475 K. Left: PDF isosurface for lithium probability density of 0.0125×10^{-6} pm^{-3} (pink) with section through Li1, Li1′, and Max [gray, ca. (0 10 47)]. Right: OPP map for the same section (e_1, e_2: orthogonal coordinates with origin at Li1; dark gray: areas of infinitely high potential). Reprinted with permission from [26] (https://pubs.acs.org/doi/10.1021/acs.chemmater.5b04608). © 2016 American Chemical Society.

the ultraslow 3D conductor γ-LiAlO$_2$ [26], both of which were analyzed using the PDF/OPP formalism. Using a 3D plot, the right part of Figure 3 vividly depicts the OPP landscape in γ-LiAlO$_2$ within the gray plane of the left part of the image. The figure was generated using the 2D-PDF routine of *CalcOPP* and *Origin* as a plotting program.

Furthermore, correlated lithium-ion migration in Li$_{10}$GeP$_2$S$_{12}$ was analyzed with *CalcOPP* [27]. The underlying measurements had however been conducted at ambient temperature and even at 10 K, which may be too low to allow ample diffusion. Thus, the results are prone to derive from static disorder rather than from migration and should be assessed with caution.
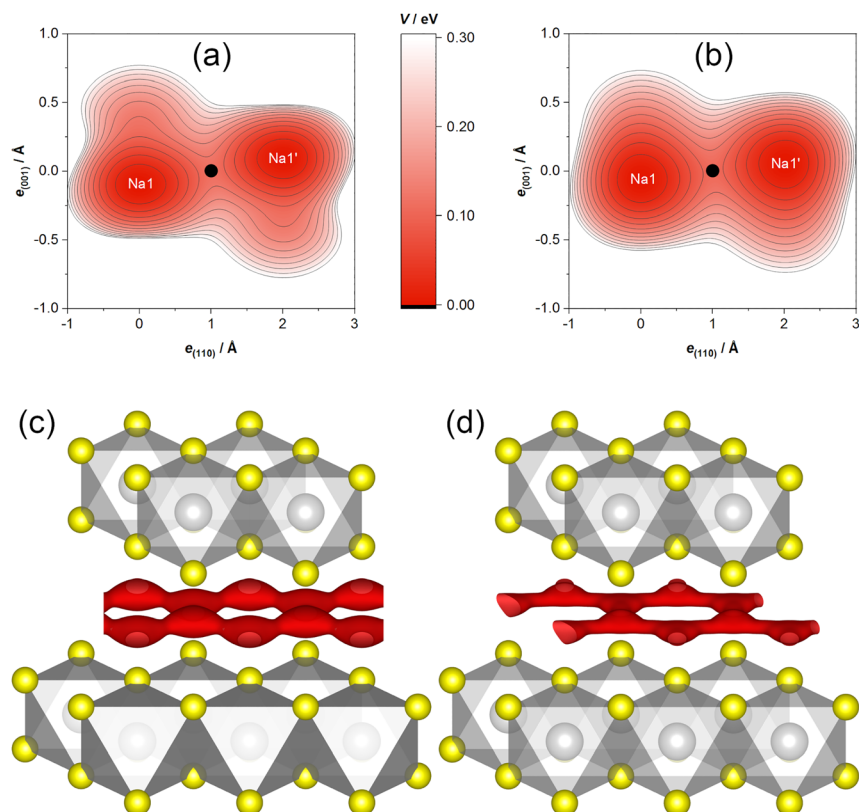

Figure 4: Sodium OPP in Na$_{0.5}$TiS$_2$-3R_1. Top: contour plot of PDF-derived OPP within a plane containing two adjacent sodium ions at (a) 600 °C and (b) 700 °C (origin at Na1, bottleneck as black dot, contours: from $V_0 = 0$ on with $\Delta V = 0.025$ eV). Bottom: isosurface plots of (c) PDF-derived and (d) SLD-derived OPP of $V = 0.15$ eV at 700 °C (atoms with covalent radii; gray: titanium, yellow: sulfide ions, red: OPP isosurface) [28]. © 2019 D. Wiedemann, E. Suard, M. Lerch (https://doi.org/10.1039/C9RA05690D). Published by The Royal Society of Chemistry. CC BY 3.0.
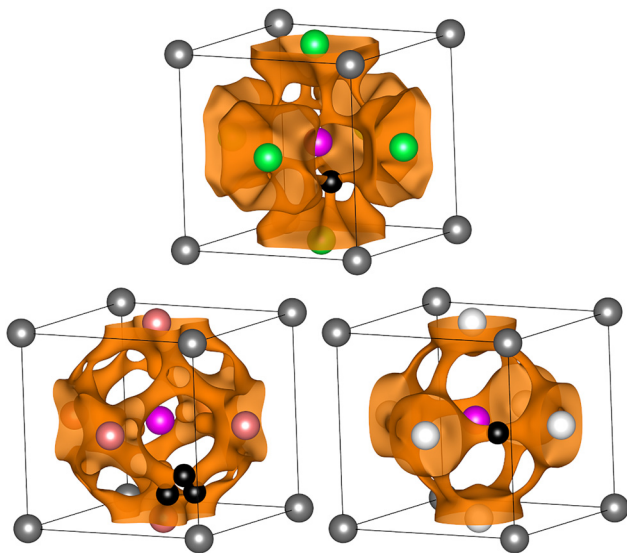
Figure 5: Anion OPPs as derived from MEM-reconstructed SLD in BaLiF$_3$ at 700 °C (top, V = 0.58 eV), in BaLiD$_3$ at 500 °C (bottom left, V = 0.37 eV), and in BaLiH$_3$ at 500 °C (bottom right, V = 0.41 eV). Orange: OPP isosurface, gray: Ba^{2+}, pink: Li$^+$, green: F$^-$, coral: D$^-$, white: H$^-$, black: exemplary bottleneck positions; ions with arbitrary radii, unit cell in black [29]. © 2019 D. Wiedemann, E. M. Heppke, A. Franz (https://doi.org/10.1002/ejic.201901232). Published by Wiley-VCH Verlag GmbH & Co. KGaA. CC BY 4.0.

As a rare example, sodium ions in the layered conductor Na$_{0.5}$TiS$_2$-3R_1 were investigated with both the PDF/OPP and the MEM/OPP formalism [28]. The results were calculated by the 2D-PDF routine of *CalcOPP* and visualized as color-coded 2D contour plots using *Origin* (see Figure 4, top) or computed with the scatterer-density routine and visualized as isosurface plots using *Vesta* (see Figure 4, bottom).

The migration of anions has sparked interest, too: In the inverse perovskites BaLiX_3 with X = F, H, D, it was also scrutinized using both formalisms [29]. Images, however, were only generated using the scatterer-density routine and *Vesta* (see Figure 5).

Finally, a work on hydride-ion conduction in the lanthanide hydride oxides LnSrLiH$_2$O$_2$ (Ln = La, Pr, Nd, Sm, Gd) [30], which also employed *CalcOPP*, should not go unmentioned, although it suffers from the same drawback as the study on Li$_{10}$GeP$_2$S$_{12}$ (vide supra).

4 Availability

Source code and released binaries are available in a repository [31] on the version-control and software-development platform *GitHub*: https://github.com/dewiedem/calcopp. It integrates with the scientific open-access repository *Zenodo* [32],

thus ensuring long-term availability and citability via a persistent digital object identifier (DOI): https://doi.org/10.5281/zenodo.2530345.

5 Conclusions

The program *CalcOPP* represents an open-source cross-platform alternative to undocumented in-house scripts for calculating OPPs from 2D/3D PDFs or MEM-reconstructed SLDs. Not only can it handle error maps, but it also takes input from and supplies output to standard crystallographic software. Written in Python 3.9 and Fortran 2018, it comes as a compressed easy-to-use executable with a CLI as well as a GUI. Its permissive MIT License allows widespread use and integration. *CalcOPP* has already been used in multiple peer-reviewed publications and can hopefully contribute to open crystallographic research in the still growing field of ion dynamics.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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Bionote

Dennis Wiedemann was born in Eutin, Germany in 1981. He obtained his B.Sc. and M.Sc. in chemistry at Freie Universität Berlin (Germany) in 2005 and 2007, respectively, specializing in inorganic molecular chemistry. His final theses dealt with lanthanoid(II) complexes as reductants and with gold(I) complexes exhibiting aurophilic interactions, respectively. He received his Dr. rer. nat. summa cum laude in 2013 from Technische Universität Berlin (Germany) after working on switchable lanthanoid and transition-metal complexes of novel pyridine-based podands under the supervision of Prof. Dr. Andreas Grohmann. It was then that he started to learn the ropes of single-crystal diffractometry.

Afterwards, he joined the group of Prof. Dr. Martin Lerch (also at Technische Universität Berlin) as a postdoctoral researcher to study ion conduction (lithium, sodium, and anions) in crystalline solids by means of X-ray and neutron powder diffraction. Modern methods in X-ray, neutron, and electron diffractometry of single crystals and powders have fascinated him ever since. His further professional interests include cheminformatics, legal aspects of chemistry, as well as equal opportunities and diversity. He joined the Deutsche Gesellschaft für Kristallographie (DGK) in 2014 and the Young Crystallographers shortly thereafter.

In 2020, he became research associate at Helmholtz-Zentrum Berlin für Materialien und Energie (Department Structure and Dynamics of Energy Materials, Prof. Dr. Susan Schorr) where he elucidated the structure of hybrid halide perovskites and studied ion migration in these materials. He is currently working as a technical consultant at GfBU-Consult Gesellschaft für Umwelt- und Managementberatung in Hoppegarten, Germany.