express: extensible, high-level workflows for swifter *ab initio* materials modeling

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Introduction

Materials computations, especially of the *ab initio* kind, are intrinsically complex. These difficulties have inspired us to develop a workflow framework, `express`, to automate long and extensive sequences of the *ab initio* calculations. Various materials properties can be computed in `express`, e.g., static equation of state, phonon density of states, thermal equation of state, and other thermodynamic properties. It helps users in the preparation of inputs, execution of simulations, and analysis of data. It also tracks the operations and steps that users performed and thus can restore interrupted or failed jobs.

Here, we present the *ab initio* results facilitated by `express` of some minerals: akimotoite, albite, bridgmanite, coesite, corundum, diopside, lime, and stishovite. They cover a wide range of crystal systems. For each material, we calculate thermodynamic properties using the quasi-harmonic approximation with three groups of exchange-correlation functionals: local-density approximation (LDA), Perdew–Burke–Ernzerhof generalized gradient approximation (PBE-GGA), and the PBE functional revised for solids (PBEsol). These results are compared to other calculations and experiments, verifying the performance of these functionals and the utility of `express`.

Besides the above advantages, `express` is also performant and extensible and runs on numerous high-performance platforms. It is open source, and everyone is welcome to use it.

Systems

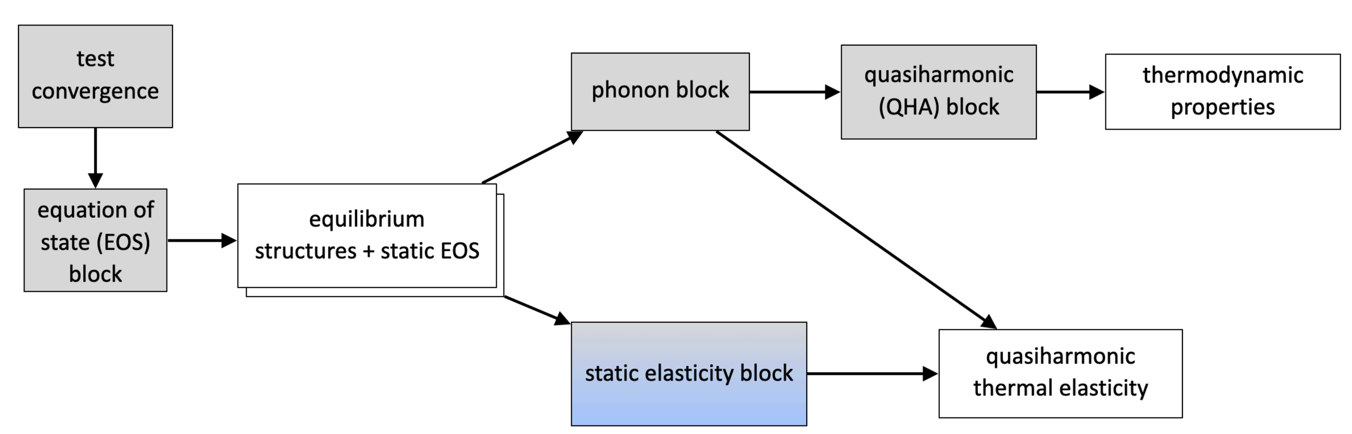
The systems and calculation parameters we investigated are listed below:

Material	Formula	Space Group	Material	Formula	Space Group
Albite	$NaAlSi_3O_8$	$P\bar{1}$	Stishovite	SiO_2	$P\frac{4_2}{m}nm$
Coesite	SiO_2	$C\frac{2}{c}$	Akimotoite	$MgSiO_3$	$R\bar{3}$
Diopside	$CaMgSi_2O_6$	$C\frac{2}{c}$	Corundum	Al_2O_3	$R\bar{3}c$
Bridgmanite	$MgSiO_3$	Pbnm	Lime	CaO	$Fm\bar{3}m$

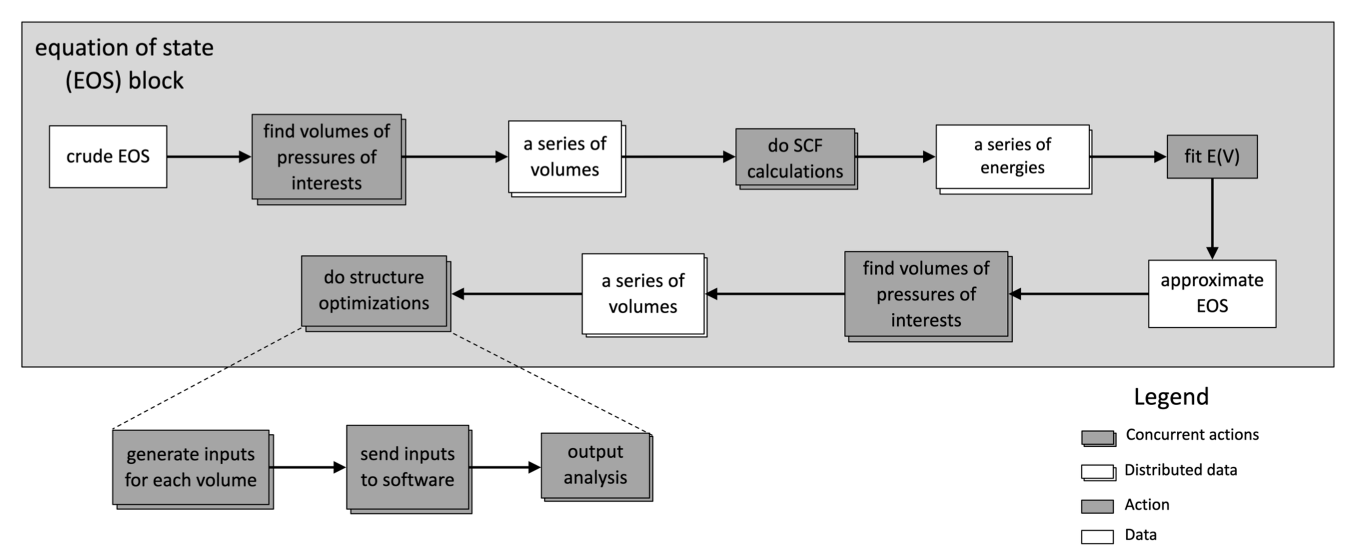
Material	Cutoff energy (Ry)			k-point mesh	q-mesh (DFPT)	q-mesh (sampling)
	LDA	PBEsol	PBE			
Albite	120	90	130	$2\times2\times2$	$2\times2\times2$	$20\times20\times20$
Coesite	110	90	130	$4\times4\times4$	$2\times2\times2$	$20\times20\times20$
Diopside	180	90	130	$4\times4\times4$	$2\times2\times2$	$20\times20\times20$
Bridgmanite	150	150	130	$6\times6\times4$	$2\times2\times2$	$20\times20\times20$
Stishovite	170	80	80	$4\times4\times6$	$2\times2\times4$	$30\times30\times30$
Akimotoite	170	90	120	$4\times4\times4$	$4\times4\times4$	$20\times20\times20$
Corundum	130	130	130	$4\times4\times4$	$4\times4\times4$	$20\times20\times20$
Lime	80	80	120	$4\times4\times4$	$4\times4\times4$	$20\times20\times20$

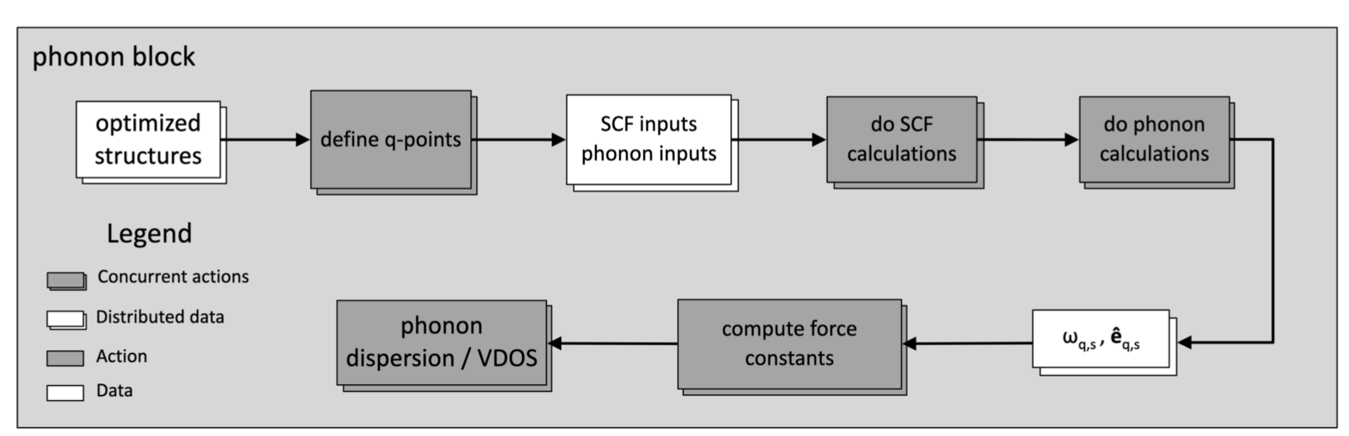
Workflows

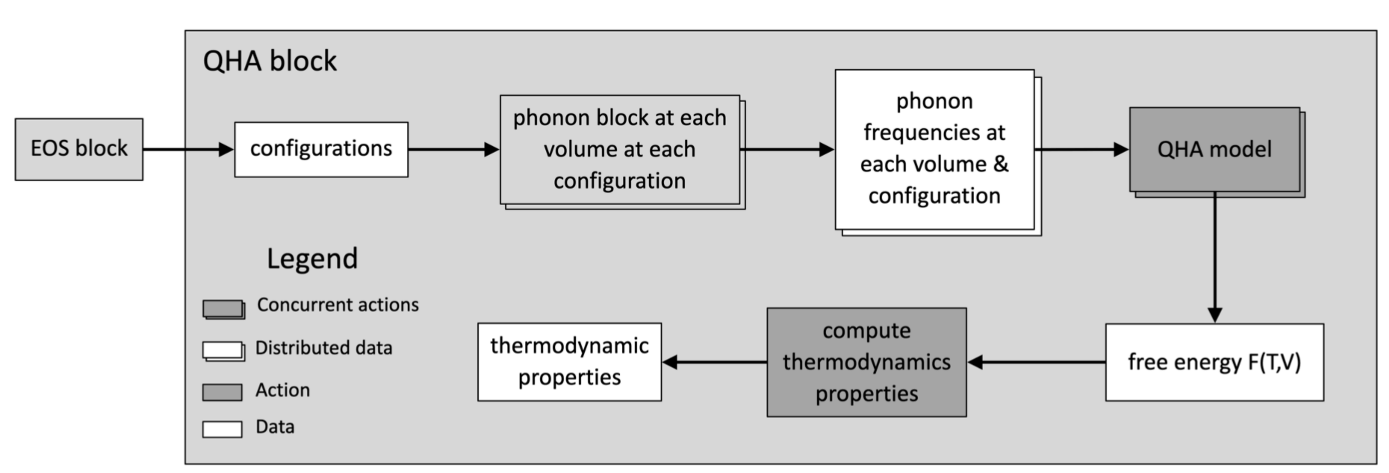
Below is a high-level overview of the workflows we included in express. Each light-gray block denotes a workflow we have and will be documented below. A white block means the results from a previous block. The static elasticity block is not currently contained in express but will be released in the near future.
The workflows are highly modularized, which can be separated, chained, and customized. Currently, we provide three major workflows: equations of state calculation, phonon spectrum calculation, and thermodynamic property calculations in the framework of the quasi-harmonic approximation (QHA).



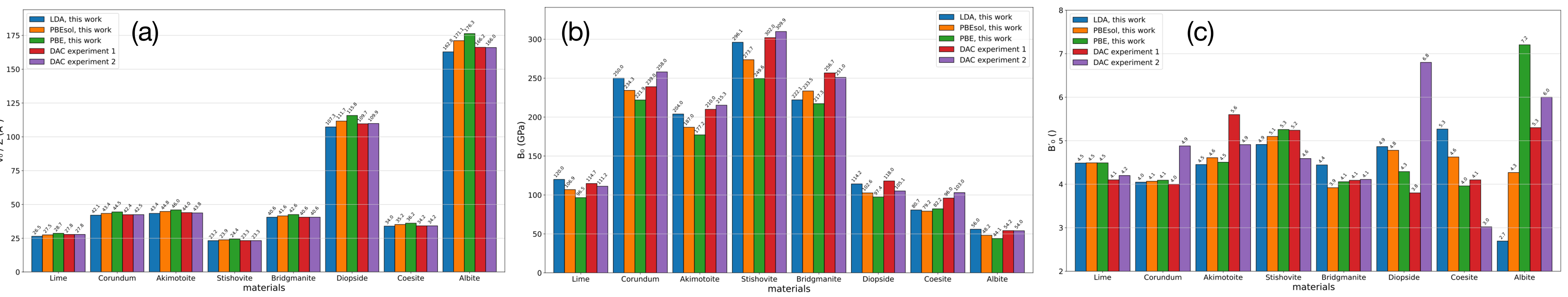
High-level schematic representation of the `express` workflows



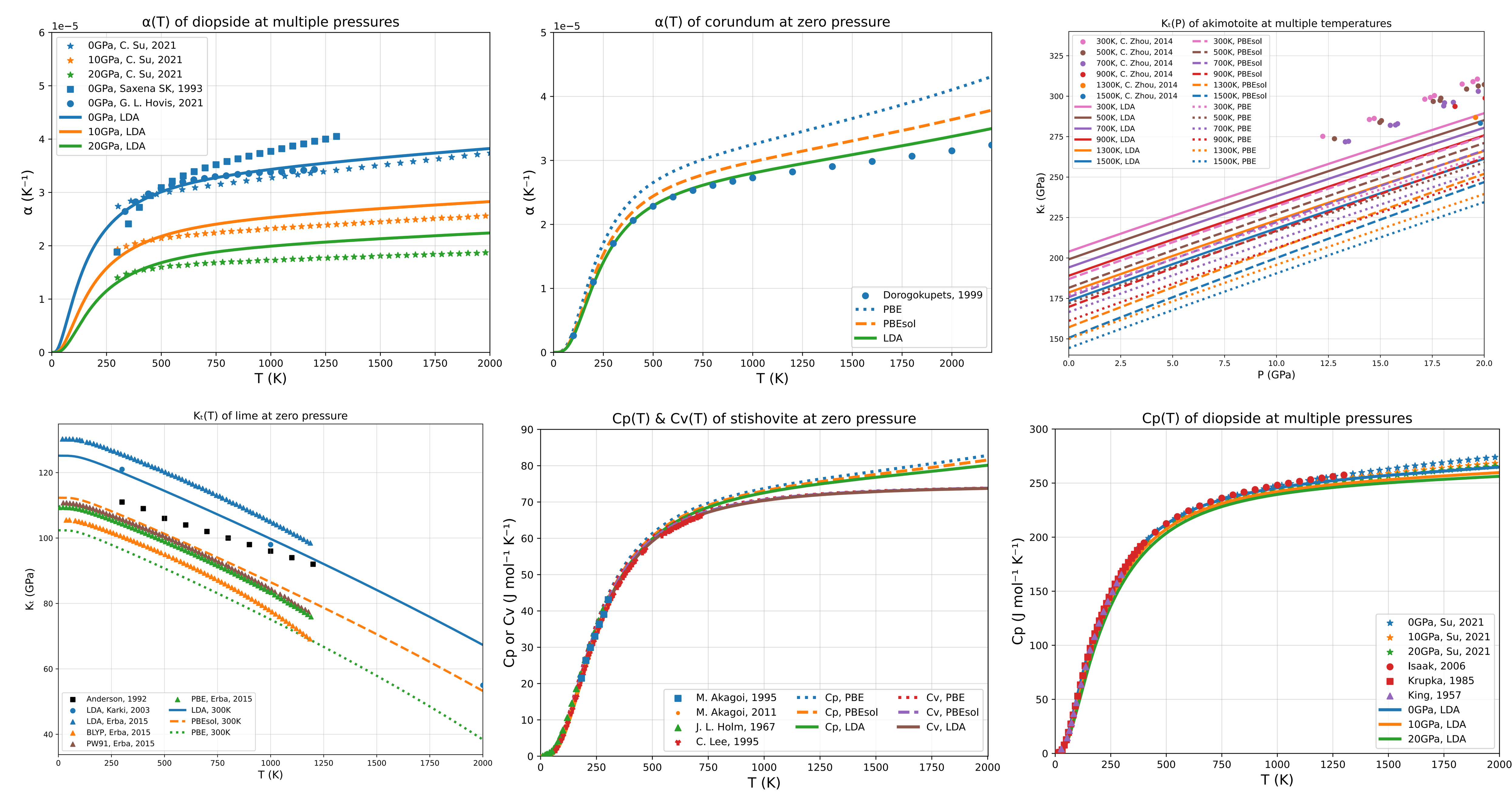




Results



Comparisons between calculated and experimental parameters (a) v0, (b) K0, and (c) K0′, at 300 K for the investigated materials, fitted by third-order Birch–Murnaghan equations of state.



Acknowledgements & References

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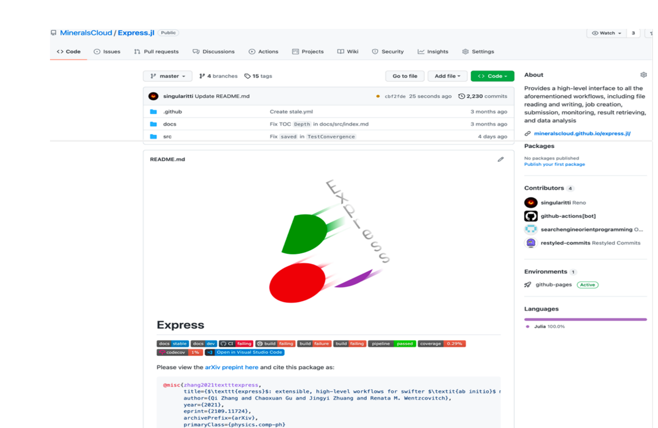

We are hosting the code on GitHub (https://github.com/MineralsCloud/Express.jl), and the preprint is on arXiv (https://arxiv.org/abs/2109.11724). You are welcome to have a look and use it.