Supplementary materials

A metadata schema for lattice thermal conductivity form first-principles calculations

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1. Metadata schema for structural optimization

Table S1 Data dictionary of metadata for structural optimization

1.1 Metadata information of structural optimization

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
1	Metadata of structural optimization	Root entity that defines the metadata of the VASP structural optimization calculation	Class	Line 2-5	M	1
2	Role name: Management information	Management information describing the data resource.	Relevancy	Management (1.2)	M	1
3	Role name: Element and structure information	Basic description of materials' crystal structure	Relevancy	Element and structure (1.3)	M	1
4	Role name: Input file information	Standard and necessary input file in VASP calculation	Relevancy	Input file (1.4)	M	1
5	Role name: Output file information	Output file containing the valuable information after a successful job	Relevancy	Output file (1.5)	M	1

1.2 Management information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
6	Management	Metadata entity for data management	Aggregate class	Line 7-14	M	1
7	Sample ID	Information required to uniquely identify a sample data resource	String	Text	M	1
8	Virtual sample name	Name given to the virtual sample	String	Text	M	1
9	Use of virtual sample preparation	Explanation for the use of sample preparation	String	Text	M	1
10	Calculation software name	Introduction for the calculation software	String	Text	M	1
11	Calculation software version	Introduction for the calculation software version	String	Text	M	1

12	Calculation date	Recording the calculation data	Date	Date	M	1
13	Calculator	Recording the calculator	String	Text	M	1
14	Associated virtual sample ID	Identification code of the previous sample if this sample is prepared on basis of the previous sample preparation	String	Text	C	1

1.3 Element and structure information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
15	Element and structure	Metadata entity for material structure	Aggregate class	Line 16-20	M	1
16	Material ID	Identification of material structure	String	Text	M	1
17	Database name	Source database of material structure	String	Text	M	1
18	Structure name	Material structure name	String	Text	M	1
19	Space group	Space group of material structure	String	Text	M	1
20	Lattice constant	Lattice constant of material structure	String	Text	M	1

1.4 Input file information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
21	Input file	Input file required for VASP calculation	Aggregate class	Line 22-25	M	1
22	INCAR	Input file containing parameter setting for VASP calculation	File	_	M	1
23	POSCAR	Input file containing structure and element information for VASP calculation	File	_	M	1
24	KPOINTS	Input file containing the sampling form and quantity of k points in Brillouin zone for VASP calculation	File	_	M	1
25	POTCAR	Input file containing pseudopotential for VASP calculation	File	_	M	1

1.5 Output file information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
26	Output file	Output file after a successful VASP calculation	Aggregate class	Line 27-36	M	1
27	CONTCAR	Output file containing structure and element information after a successful VASP calculation	File	_	M	1
28	DOSCAR	Contains the density of states	File	_	M	1
29	EIGENVAL	Contains the Kohn-Sham-eigenvalues for all k-points at the end of the simulation.	File	_	M	1
30	IBZKPT	Is compatible with the KPOINTS file and is generated if the automatic k-mesh generation is selected in the KPOINTS file.	File	_	M	1
31	OSZICAR	Information about convergence speed and about the current step	File	_	M	1
32	OUTCAR	Gives detailed output of a VASP run	File	_	M	1
33	PCDAT	Contains the pair correlation function.	File	_	M	1
34	vasprun.xml	The output file in xml format after a successful VASP job.	File	_	M	1
35	XDATCAR	Contains the ionic configuration of the system after a given number of ionic steps	File	_	M	1
36	vasp.out	Output file contain the calculation process	File	_	M	1

2. Metadata schema of force constants calculation

Table S2 Data dictionary of metadata for force constants calculation

2.1 Metadata information of force constants calculation

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
1	Metadata of force constants calculation	Root entity that defines the metadata of the force constants calculation	Class	Line 2-4	M	1
2	Role name: Management information	Management information describing the data resource.	Relevancy	Management (2.2)	M	1
3	Role name: Input file information	Standard and necessary input file in VASP calculation	Relevancy	Input file (2.3)	M	1
4	Role name: Output file information	Standard and necessary output file in VASP calculation	Relevancy	Output file (2.4)	M	1

2.2 Management information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
5	Management	Metadata entity for data management	Aggregate class	Line 6-12	M	1
6	Source data ID	Identification of the source data	String	Text	M	1
7	Virtual characterization name	Name given to the virtual characterization	String	Text	M	1
8	Calculation software name	Introduction for the calculation software	String	Text	M	1
9	Calculation software version	Introduction for the calculation software version	String	Text	M	1
10	Calculation date	Recording the calculation data	Date	Date	M	1
11	Calculator	Recording the calculator	String	Text	M	1
12	Associated virtual sample ID	Identification code of sample source for characterization	String	Text	M	1

2.3 Input file information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
13	Input file	Input file required for VASP calculation	Aggregate class	Line 14-17	M	1
14	INCAR	Input file containing parameter setting for VASP calculation	File	_	M	1
15	POSCAR	Input file containing structure and element information for VASP calculation	File	_	M	1..n
16	KPOINTS	Input file containing the sampling form and quantity of k points in Brillouin zone for VASP calculation	File	_	M	1
17	POTCAR	Input file containing pseudopotential for VASP calculation	File	_	M	1

2.4 Output file information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
18	Output file	Output file after a successful VASP calculation	Aggregate class	Line 19 -30	M	1
19	vasprun.xml	Output file used for force analysis after a successful VASP calculation	File	_	M	1..n
20	FORCE_CONSTANTS	Second-order force constants file created by Phonopy	File	-	C	1
21	FORCE_CONSTANTS_3RD	Third-order force constants file created by Thirdorder	File	-	C	1
22	CONTCAR	Output file containing structure and element information after a successful VASP calculation	File	_	M	1..n
23	DOSCAR	Contains the density of states	File	_	M	1..n
24	EIGENVAL	Contains the Kohn-Sham-eigenvalues for all k-points at the end of the simulation.	File	_	M	1..n
25	IBZKPT	Is compatible with the KPOINTS file and is generated if the automatic k-mesh generation is selected in the KPOINTS file.	File	_	M	1..n

26	OSZICAR	Information about convergence speed and about the current step	File	_	M	1..n
27	OUTCAR	Gives detailed output of a VASP run	File	_	M	1..n
28	PCDAT	Contains the pair correlation function.	File	_	M	1..n
29	XDATCAR	Contains the ionic configuration of the system after a given number of ionic steps	File	_	M	1..n
30	vasp.out	Output file contain the calculation process	File	_	M	1..n

3. Metadata schema of phonon thermal conductivity calculation

Table S3 Data dictionary of metadata for phonon thermal conductivity calculation

3.1 Metadata information of phonon thermal conductivity calculation

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
1	Metadata of phonon thermal conductivity calculation	Root entity that defines the metadata of the force constants calculation	Class	Line 2-4	M	1
2	Role name: Management information	Management information describing the data resource.	Relevancy	Management (3.2)	M	1
3	Role name: Input file information	Standard and necessary input file in ShengBTE calculation	Relevancy	Input file (3.3)	M	1
4	Role name: Output file information	Output file containing the phonon thermal conductivity	Relevancy	Output file (3.4)	M	1

3.2 Management information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
5	Management	Metadata entity for data management	Aggregate class	Line 6-12	M	1
6	Data ID	Identification of the derived data	String	Text	M	1
7	Calculation name	Name given to the calculation	String	Text	M	1
8	Calculation software name	Introduction for the calculation software	String	Text	M	1
9	Calculation software version	Introduction for the calculation software version	String	Text	M	1
10	Calculation date	Recording the calculation data	Date	Date	M	1
11	Calculator	Recording the calculator	String	Text	M	1
12	Associated source data ID	Identification code of source data	String	Text	M	2

3.3 Input file information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
13	Input file	Input file required for ShengBTE calculation	Aggregate class	Line 14-16	M	1
14	CONTROL	Input file describing the system to be studied and specify a set of parameters and flags controlling execution.	File	_	M	1
15	FORCE_CONSTANTS_2ND	Second-order force constants	File	_	M	1
16	FORCE_CONSTANTS_3ND	Third-order force constants	File	_	M	1

3.4 Output file information

Serial number	Name	Definition	Data type	Range	Restriction	Maximum number of occurrences
17	Output file	Output file after a successful ShengBTE calculation	Aggregate class	Line 18-39	M	1
18	BTE.KappaTensorVsT_CONV	Total converged thermal conductivity tensor in unit of W/(m K) as a function of T (1st column).	File	_	M	1
19	BTE.KappaTensorVsT_RTA	Total thermal conductivity tensor in unit of W/(m K) in the Relaxation Time Approximation as a function of T.	File	_	M	1
20	BTE.KappaTensorVsT_sg	Thermal conductivity tensor per unit of mean free path in the small-grain limit	File	_	M	1
21	BTE.cvVsT	Specific heat of the system	File	_	M	1
22	BTE.dos	Phonon density of states	File	_	M	1
23	BTE.gruneisen	Grüneisen parameter for each irreducible q point	File	_	M	1

		and phonon band				
24	BTE.gruneisenVsT_total	Total Grüneisen parameter obtained as a weighted sum of the mode contributions as a function of T	File	_	M	1
25	BTE.omega	Phonon angular frequencies	File	_	M	1
26	BTE.P3	Volume in phase space available for three-phonon processes	File	_	M	1
27	BTE.P3_minus	_	File	_	M	1
28	BTE.P3_minus_total	_	File	_	M	1
29	BTE.P3_plus	_	File	_	M	1
30	BTE.P3_plus_total	_	File	_	M	1
31	BTE.P3_total	Sum of all the contributions in `BTE.P3`	File	_	M	1
32	BTE.pdos	Phonon density of states projected on each atom	File	_	M	1
33	BTE.qpoints	Gives q points in the irreducible wedge of Brillouin zone (BZ)	File	_	M	1
34	BTE.qpoints_full	Lists all q points in `ngrid(1)` x `ngrid(2)` x `ngrid(3)` &Gamma-centered regular grid.	File	_	M	1
35	BTE.ReciprocalLatticeVectors	Three reciprocal lattice basis vectors	File	_	M	1
36	BTE.v	Group velocities of those modes	File	_	M	1
37	BTE.v_full	Group velocities of all modes for all points	File	_	M	1
38	BTE.w_boundary	Boundary scattering rate	File	_	M	1
39	BTE.w_isotopic	Isotopic scattering rate	File	_	M	1

Table S4 Metadata example table for Si structural optimization via VASP

Metadata item		Metadata record
Management information	Sample ID	SI-001
	Virtual sample name	Si
	Use of virtual sample preparation	Structural optimization
	Calculation software name	VASP
	Calculation software version	VASP.5.4.4
	Calculation date	07.18.2020
	Calculator	Yongchao Rao
	Associated virtual sample ID	_
Element and structure information	Material ID	mp-149
	Database name	Materials Project
	Structure name	Si
	Space group	Fd-3m
	Lattice constant	a=b=c=3.867 Å, α=β=γ=60°
Input file information	INCAR	File
	POSCAR	File
	KPOINTS	File
	POTCAR	File
Output file information	CONTCAR	File
	DOSCAR	File
	EIGENVAL	File
	IBZKPT	File
	OSZICAR	File
	OUTCAR	File
	PCDAT	File
	vasprun.xml	File
	XDATCAR	File
	vasp.out	File

Table S5 Metadata example table for Si force constants calculation via VASP

Metadata item		Metadata record
Management information	Source data ID	SD-001
	Virtual characterization name	Force constants calculation
	Calculation software name	VASP, Phonopy/Thirdorder
	Calculation software version	VASP.5.4.4, Phonopy.2.9.1, Thirdorder v1.0.0
	Calculation date	04.21.2021
	Calculator	Yongchao Rao
	Associated virtual sample ID	SI-001
Input file information	INCAR	File
	POSCAR	File
	KPOINTS	File
	POTCAR	File
Output file information	vasprun.xml	File
	FORCE_CONSTANTS	File
	FORCE_CONSTANTS_3RD	File
	CONTCAR	File
	DOSCAR	File
	EIGENVAL	File
	IBZKPT	File
	OSZICAR	File
	OUTCAR	File
	PCDAT	File
	XDATCAR	File
	vasp.out	File

Table S6 Metadata example table for Si phonon thermal conductivity calculation via ShengBTE

Metadata item		Metadata record
Management information	Data ID	PD-001
	Calculation name	Phonon thermal conductivity calculation
	Calculation software name	ShengBTE
	Calculation software version	ShengBTE-v1.1.1
	Calculation date	04.21.2021
	Calculator	Yongchao Rao
	Associated source data ID	SD-001 & SD-002
Input file information	CONTROL	File
	FORCE_CONSTANTS_2ND (VASP) / espresso.ifc2 (Quantum Espresso)	File
	FORCE_CONSTANTS_3ND	File
Output file information	BTE.KappaTensorVsT_CONV	File
	BTE.KappaTensorVsT_RTA	File
	BTE.KappaTensorVsT_sg	File
	BTE.cvVsT	File
	BTE.dos	File
	BTE.gruneisen	File
	BTE.gruneisenVsT_total	File
	BTE.omega	File
	BTE.P3	File
	BTE.P3_minus	File
	BTE.P3_minus_total	File
	BTE.P3_plus	File
	BTE.P3_plus_total	File
	BTE.P3_total	File
	BTE.pdos	File
	BTE.qpoints	File
	BTE.qpoints_full	File
	BTE.ReciprocalLatticeVectors	File
	BTE.v	File
	BTE.v_full	File
	BTE.w_boundary	File
	BTE.w_isotopic	File

Table S7 Metadata example table for Si structural optimization via Quantum Espresso

Metadata item		Metadata record
Management information	Sample ID	SI-001
	Virtual sample name	Si
	Use of virtual sample preparation	Structural optimization
	Calculation software name	Quantum Espresso
	Calculation software version	QE v.6.7
	Calculation date	08.22.2020
	Calculator	Yongchao Rao
	Associated virtual sample ID	_
Element and structure information	Material ID	mp-149
	Database name	Materials Project
	Structure name	Si
	Space group	Fd-3m
	Lattice constant	a=b=c=3.867 Å, α=β=γ=60°
Input file information	vc-relax.in	File
	Si.pbe-n-kjpaw_psl.1.0.0.UPF	File
Output file information	vc-relax.out	File

Table S8.1 Metadata example table for Si second-order force constants calculation via Quantum Espresso

Metadata item		Metadata record
Management information	Source data ID	SD-001
	Virtual characterization name	Force constants calculation
	Calculation software name	Quantum Espresso
	Calculation software version	QE v.6.7
	Calculation date	11.01.2021
	Calculator	Yongchao Rao
	Associated virtual sample ID	SI-001
Input file information	scf.in	File
	ph.in	File
	q2r.in	File
	Si.pbe-n-kjpaw_psl.1.0.0.UPF	File
Output file information	scf.out	File
	ph.out	File
	q2r.out	File
	espresso.ifc2	File
	Si.dyn0	File
	Si.dyn1	File
	Si.dyn2	File
	Si.dyn3	File
	Si.dyn4	File
	Si.dyn5	File
	Si.dyn6	File
	Si.dyn7	File
	Si.dyn8	File
	Si.xml	File

Table S8.2 Metadata example table for Si third-order force constants calculation via Quantum Espresso

Metadata item		Metadata record
Management information	Source data ID	SD-002
	Virtual characterization name	Force constants calculation
	Calculation software name	Quantum Espresso
	Calculation software version	QE v.6.7
	Calculation date	11.01.2021
	Calculator	Yongchao Rao
	Associated virtual sample ID	SI-001
Input file information	scf.in	File
	scf_sc.in	File
	DISP.scf_sc.in	File
	Si.pbe-n-kjpaw_psl.1.0.0.UPF	File
Output file information	DISP.scf_sc.in.out	File
	FORCE_CONSTANTS_3RD	File