INCAR\_SYSTEM: {{ INCAR\_SYSTEM }}

INCAR\_Source: {{ INCAR\_Source }}

INCAR\_ISTART: {{ INCAR\_ISTART }}

INCAR\_PREC: {{ INCAR\_PREC }}

INCAR\_NBANDS: {{ INCAR\_NBANDS }}

INCAR\_EDIFF: {{ INCAR\_EDIFF }}

INCAR\_EDIFFG: {{ INCAR\_EDIFFG }}

INCAR\_LREAL: {{ INCAR\_LREAL }}

INCAR\_GGA: {{ INCAR\_GGA }}

INCAR\_ALGO: {{ INCAR\_ALGO }}

INCAR\_NELMIN: {{ INCAR\_NELMIN }}

INCAR\_ISPIN: {{ INCAR\_ISPIN }}

INCAR\_LMAXMIX: {{ INCAR\_LMAXMIX }}

INCAR\_1: {{ INCAR\_1 }}

INCAR\_3: {{ INCAR\_3 }}

INCAR\_5\_6: {{ INCAR\_5\_6 }}

INCAR\_7\_8: {{ INCAR\_7\_8 }}

INCAR\_PSTRESS: {{ INCAR\_PSTRESS }}

INCAR\_2: {{ INCAR\_2 }}

INCAR\_ISYM: {{ INCAR\_ISYM }}

INCAR\_EFERMI: {{ INCAR\_EFERMI }}

INCAR\_LWAVE: {{ INCAR\_LWAVE }}

INCAR\_LCHARG: {{ INCAR\_LCHARG }}

INCAR\_LVTOT: {{ INCAR\_LVTOT }}

INCAR\_LKPOINTS\_OPT: {{ INCAR\_LKPOINTS\_OPT }}

INCAR\_LELF: {{ INCAR\_LELF }}

INCAR\_LAECHG: {{ INCAR\_LAECHG }}

INCAR\_NPAR: {{ INCAR\_NPAR }}

INCAR\_LPLANE: {{ INCAR\_LPLANE }}

INCAR\_RWIGS: {{ INCAR\_RWIGS }}

INCAR\_ISMEAR: {{ INCAR\_ISMEAR }}

INCAR\_SIGMA: {{ INCAR\_SIGMA }}

POTCAR\_PP0: {{ POTCAR\_PP0 }}

POTCAR\_Atom0: {{ POTCAR\_Atom0 }}

POTCAR\_Ne0: {{ POTCAR\_Ne0 }}

POTCAR\_PP1: {{ POTCAR\_PP1 }}

POTCAR\_Atom1: {{ POTCAR\_Atom1 }}

POTCAR\_Ne1: {{ POTCAR\_Ne1 }}

POTCAR\_nPPTypes: {{ POTCAR\_nPPTypes }}

POSCAR: {{ POSCAR }}

CONTCAR: {{ CONTCAR }}

OUTCAR\_binary: {{ OUTCAR\_binary }}

OUTCAR\_compiler: {{ OUTCAR\_compiler }}

OUTCAR\_mpi: {{ OUTCAR\_mpi }}

OUTCAR\_ncores\_k: {{ OUTCAR\_ncores\_k }}

OUTCAR\_ncores\_band: {{ OUTCAR\_ncores\_band }}

OUTCAR\_SYSTEM: {{ OUTCAR\_SYSTEM }}

OUTCAR\_ISTART: {{ OUTCAR\_ISTART }}

OUTCAR\_PREC: {{ OUTCAR\_PREC }}

OUTCAR\_NBANDS: {{ OUTCAR\_NBANDS }}

OUTCAR\_EDIFF: {{ OUTCAR\_EDIFF }}

OUTCAR\_EDIFFG: {{ OUTCAR\_EDIFFG }}

OUTCAR\_LREAL: {{ OUTCAR\_LREAL }}

OUTCAR\_GGA: {{ OUTCAR\_GGA }}

OUTCAR\_ALGO: {{ OUTCAR\_ALGO }}

OUTCAR\_NELMIN: {{ OUTCAR\_NELMIN }}

OUTCAR\_ISPIN: {{ OUTCAR\_ISPIN }}

OUTCAR\_LMAXMIX: {{ OUTCAR\_LMAXMIX }}

OUTCAR\_PSTRESS: {{ OUTCAR\_PSTRESS }}

OUTCAR\_ISYM: {{ OUTCAR\_ISYM }}

OUTCAR\_EFERMI: {{ OUTCAR\_EFERMI }}

OUTCAR\_LWAVE: {{ OUTCAR\_LWAVE }}

OUTCAR\_LCHARG: {{ OUTCAR\_LCHARG }}

OUTCAR\_LVTOT: {{ OUTCAR\_LVTOT }}

OUTCAR\_LKPOINTS\_OPT: {{ OUTCAR\_LKPOINTS\_OPT }}

OUTCAR\_LELF: {{ OUTCAR\_LELF }}

OUTCAR\_LAECHG: {{ OUTCAR\_LAECHG }}

OUTCAR\_NPAR: {{ OUTCAR\_NPAR }}

OUTCAR\_LPLANE: {{ OUTCAR\_LPLANE }}

OUTCAR\_RWIGS: {{ OUTCAR\_RWIGS }}

OUTCAR\_ISMEAR: {{ OUTCAR\_ISMEAR }}

OUTCAR\_SIGMA: {{ OUTCAR\_SIGMA }}

OUTCAR\_NWRITE: {{ OUTCAR\_NWRITE }}

OUTCAR\_ICHARG: {{ OUTCAR\_ICHARG }}

OUTCAR\_LNONCOLLINEAR: {{ OUTCAR\_LNONCOLLINEAR }}

OUTCAR\_LSORBIT: {{ OUTCAR\_LSORBIT }}

OUTCAR\_INIWAV: {{ OUTCAR\_INIWAV }}

OUTCAR\_LASPH: {{ OUTCAR\_LASPH }}

OUTCAR\_ENCUT: {{ OUTCAR\_ENCUT }}

OUTCAR\_ENINI: {{ OUTCAR\_ENINI }}

OUTCAR\_ENAUG: {{ OUTCAR\_ENAUG }}

OUTCAR\_NELM: {{ OUTCAR\_NELM }}

OUTCAR\_NELMDL: {{ OUTCAR\_NELMDL }}

OUTCAR\_NLSPLINE: {{ OUTCAR\_NLSPLINE }}

OUTCAR\_LCOMPAT: {{ OUTCAR\_LCOMPAT }}

OUTCAR\_GGA\_COMPAT: {{ OUTCAR\_GGA\_COMPAT }}

OUTCAR\_LMAXPAW: {{ OUTCAR\_LMAXPAW }}

OUTCAR\_VOSKOWN: {{ OUTCAR\_VOSKOWN }}

OUTCAR\_ROPT: {{ OUTCAR\_ROPT }}

OUTCAR\_NSW: {{ OUTCAR\_NSW }}

OUTCAR\_NBLOCK: {{ OUTCAR\_NBLOCK }}

OUTCAR\_KBLOCK: {{ OUTCAR\_KBLOCK }}

OUTCAR\_IBRION: {{ OUTCAR\_IBRION }}

OUTCAR\_NFREE: {{ OUTCAR\_NFREE }}

OUTCAR\_ISIF: {{ OUTCAR\_ISIF }}

OUTCAR\_IWAVPR: {{ OUTCAR\_IWAVPR }}

OUTCAR\_LCORR: {{ OUTCAR\_LCORR }}

OUTCAR\_POTIM: {{ OUTCAR\_POTIM }}

OUTCAR\_TEIN: {{ OUTCAR\_TEIN }}

OUTCAR\_TEBEG: {{ OUTCAR\_TEBEG }}

OUTCAR\_TEEND: {{ OUTCAR\_TEEND }}

OUTCAR\_SMASS: {{ OUTCAR\_SMASS }}

OUTCAR\_\_Omega\_: {{ OUTCAR\_\_Omega\_ }}

OUTCAR\_SCALEE: {{ OUTCAR\_SCALEE }}

OUTCAR\_NPACO: {{ OUTCAR\_NPACO }}

OUTCAR\_APACO: {{ OUTCAR\_APACO }}

OUTCAR\_POMASS: {{ OUTCAR\_POMASS }}

OUTCAR\_ZVAL: {{ OUTCAR\_ZVAL }}

OUTCAR\_VCA: {{ OUTCAR\_VCA }}

OUTCAR\_NELECT: {{ OUTCAR\_NELECT }}

OUTCAR\_NUPDOWN: {{ OUTCAR\_NUPDOWN }}

OUTCAR\_EMIN: {{ OUTCAR\_EMIN }}

OUTCAR\_EMAX: {{ OUTCAR\_EMAX }}

OUTCAR\_METHOD: {{ OUTCAR\_METHOD }}

OUTCAR\_IALGO: {{ OUTCAR\_IALGO }}

OUTCAR\_LDIAG: {{ OUTCAR\_LDIAG }}

OUTCAR\_LSUBROT: {{ OUTCAR\_LSUBROT }}

OUTCAR\_TURBO: {{ OUTCAR\_TURBO }}

OUTCAR\_IRESTART: {{ OUTCAR\_IRESTART }}

OUTCAR\_NREBOOT: {{ OUTCAR\_NREBOOT }}

OUTCAR\_NMIN: {{ OUTCAR\_NMIN }}

OUTCAR\_EREF: {{ OUTCAR\_EREF }}

OUTCAR\_IMIX: {{ OUTCAR\_IMIX }}

OUTCAR\_AMIX: {{ OUTCAR\_AMIX }}

OUTCAR\_BMIX: {{ OUTCAR\_BMIX }}

OUTCAR\_AMIX\_MAG: {{ OUTCAR\_AMIX\_MAG }}

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OUTCAR\_WC: {{ OUTCAR\_WC }}

OUTCAR\_INIMIX: {{ OUTCAR\_INIMIX }}

OUTCAR\_MIXPRE: {{ OUTCAR\_MIXPRE }}

OUTCAR\_MAXMIX: {{ OUTCAR\_MAXMIX }}

OUTCAR\_WEIMIN: {{ OUTCAR\_WEIMIN }}

OUTCAR\_EBREAK: {{ OUTCAR\_EBREAK }}

OUTCAR\_DEPER: {{ OUTCAR\_DEPER }}

OUTCAR\_TIME: {{ OUTCAR\_TIME }}

OUTCAR\_A\_a\_u\_: {{ OUTCAR\_A\_a\_u\_ }}

OUTCAR\_a\_u\_\_A\_eV\_Ry: {{ OUTCAR\_a\_u\_\_A\_eV\_Ry }}

OUTCAR\_A: {{ OUTCAR\_A }}

OUTCAR\_LDOWNSAMPLE: {{ OUTCAR\_LDOWNSAMPLE }}

OUTCAR\_LVHAR: {{ OUTCAR\_LVHAR }}

OUTCAR\_LORBIT: {{ OUTCAR\_LORBIT }}

OUTCAR\_LMONO: {{ OUTCAR\_LMONO }}

OUTCAR\_LDIPOL: {{ OUTCAR\_LDIPOL }}

OUTCAR\_IDIPOL: {{ OUTCAR\_IDIPOL }}

OUTCAR\_EPSILON: {{ OUTCAR\_EPSILON }}

OUTCAR\_LEXCH: {{ OUTCAR\_LEXCH }}

OUTCAR\_LIBXC: {{ OUTCAR\_LIBXC }}

OUTCAR\_LHFCALC: {{ OUTCAR\_LHFCALC }}

OUTCAR\_LHFONE: {{ OUTCAR\_LHFONE }}

OUTCAR\_AEXX: {{ OUTCAR\_AEXX }}

OUTCAR\_LEPSILON: {{ OUTCAR\_LEPSILON }}

OUTCAR\_LRPA: {{ OUTCAR\_LRPA }}

OUTCAR\_LNABLA: {{ OUTCAR\_LNABLA }}

OUTCAR\_LVEL: {{ OUTCAR\_LVEL }}

OUTCAR\_CSHIFT: {{ OUTCAR\_CSHIFT }}

OUTCAR\_OMEGAMAX: {{ OUTCAR\_OMEGAMAX }}

OUTCAR\_DEG\_THRESHOLD: {{ OUTCAR\_DEG\_THRESHOLD }}

OUTCAR\_RTIME: {{ OUTCAR\_RTIME }}

OUTCAR\_\_WPLASMAI: {{ OUTCAR\_\_WPLASMAI }}

OUTCAR\_DFIELD: {{ OUTCAR\_DFIELD }}

OUTCAR\_KPOINTS\_OPT\_MODE: {{ OUTCAR\_KPOINTS\_OPT\_MODE }}

OUTCAR\_ORBITALMAG: {{ OUTCAR\_ORBITALMAG }}

OUTCAR\_LCHIMAG: {{ OUTCAR\_LCHIMAG }}

OUTCAR\_DQ: {{ OUTCAR\_DQ }}

OUTCAR\_LLRAUG: {{ OUTCAR\_LLRAUG }}

OUTCAR\_LBONE: {{ OUTCAR\_LBONE }}

OUTCAR\_LVGVCALC: {{ OUTCAR\_LVGVCALC }}

OUTCAR\_LVGVAPPL: {{ OUTCAR\_LVGVAPPL }}

OUTCAR\_RANDOM\_GENERATOR: {{ OUTCAR\_RANDOM\_GENERATOR }}

OUTCAR\_PCG\_SEED: {{ OUTCAR\_PCG\_SEED }}

OUTCAR\_EF: {{ OUTCAR\_EF }}

OUTCAR\_E\_fermi: {{ OUTCAR\_E\_fermi }}

OUTCAR\_Vcore: {% for item in OUTCAR\_Vcore %}
- {{ item }}
{% endfor %}

OUTCAR\_FreeEnergy: {% for item in OUTCAR\_FreeEnergy %}
- {{ item }}
{% endfor %}

OUTCAR\_TOTEN: {{ OUTCAR\_TOTEN }}

OUTCAR\_TOTEN\_without\_entropy: {{ OUTCAR\_TOTEN\_without\_entropy }}

OUTCAR\_TOTEN\_zero\_sigma: {{ OUTCAR\_TOTEN\_zero\_sigma }}

OUTCAR\_EF\_BZINTS\_: {{ OUTCAR\_EF\_BZINTS\_ }}

OUTCAR\_FinalCharges: {% for item in OUTCAR\_FinalCharges %}
- {{ item }}
{% endfor %}

OUTCAR\_nIon: {{ OUTCAR\_nIon }}

OUTCAR\_IsHF: {{ OUTCAR\_IsHF }}

OUTCAR\_IsMETAGGA: {{ OUTCAR\_IsMETAGGA }}

OUTCAR\_Total\_CPU\_time: {{ OUTCAR\_Total\_CPU\_time }}

OUTCAR\_User\_time: {{ OUTCAR\_User\_time }}

OUTCAR\_System\_time: {{ OUTCAR\_System\_time }}

OUTCAR\_Elapsed\_time: {{ OUTCAR\_Elapsed\_time }}

DOSCAR\_NCDIJ: {{ DOSCAR\_NCDIJ }}

DOSCAR\_POTIM: {{ DOSCAR\_POTIM }}

DOSCAR\_cry: {{ DOSCAR\_cry }}

DOSCAR\_SampleName: {{ DOSCAR\_SampleName }}

DOSCAR\_IsSpinPolarized: {{ DOSCAR\_IsSpinPolarized }}

DOSCAR\_ISPIN: {{ DOSCAR\_ISPIN }}

DOSCAR\_SpinOrbit: {{ DOSCAR\_SpinOrbit }}

DOSCAR\_IsNonCollinear: {{ DOSCAR\_IsNonCollinear }}

DOSCAR\_ks: {{ DOSCAR\_ks }}

DOSCAR\_nions\_with\_empty: {{ DOSCAR\_nions\_with\_empty }}

DOSCAR\_nions: {{ DOSCAR\_nions }}

DOSCAR\_atom\_types: {% for item in DOSCAR\_atom\_types %}
- {{ item }}
{% endfor %}

DOSCAR\_atom\_sites: {% for item in DOSCAR\_atom\_sites %}
- {{ item }}
{% endfor %}

DOSCAR\_natom\_types: {{ DOSCAR\_natom\_types }}

DOSCAR\_natom\_sites: {{ DOSCAR\_natom\_sites }}

DOSCAR\_Vcell: {{ DOSCAR\_Vcell }}

DOSCAR\_a: {{ DOSCAR\_a }}

DOSCAR\_b: {{ DOSCAR\_b }}

DOSCAR\_c: {{ DOSCAR\_c }}

DOSCAR\_EF: {{ DOSCAR\_EF }}

DOSCAR\_Efermi: {{ DOSCAR\_Efermi }}

DOSCAR\_TEBEG: {{ DOSCAR\_TEBEG }}

DOSCAR\_include\_PODS: {{ DOSCAR\_include\_PODS }}

DOSCAR\_Emax: {{ DOSCAR\_Emax }}

DOSCAR\_Emin: {{ DOSCAR\_Emin }}

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DOSCAR\_E: {% for item in DOSCAR\_E %}
- {{ item }}
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DOSCAR\_TotalDOS: {% for item in DOSCAR\_TotalDOS %}
- {{ item }}
{% endfor %}

DOSCAR\_TotalDOSup: {% for item in DOSCAR\_TotalDOSup %}
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{% endfor %}

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- {{ item }}
{% endfor %}

DOSCAR\_Nedn: {{ DOSCAR\_Nedn }}

DOSCAR\_npdos: {{ DOSCAR\_npdos }}

DOSCAR\_lmlabels: {% for item in DOSCAR\_lmlabels %}
- {{ item }}
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DOSCAR\_PDOS\_list\_Zn: {% for item in DOSCAR\_PDOS\_list\_Zn %}
- {{ item }}
{% endfor %}

DOSCAR\_PDOS\_list\_O: {% for item in DOSCAR\_PDOS\_list\_O %}
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{% endfor %}

DOSCAR\_PDOS\_atom\_list: {% for item in DOSCAR\_PDOS\_atom\_list %}
- {{ item }}
{% endfor %}

DOSCAR\_sumDOS\_list: {% for item in DOSCAR\_sumDOS\_list %}
- {{ item }}
{% endfor %}

DOSCAR\_data\_list: {% for item in DOSCAR\_data\_list %}
- {{ item }}
{% endfor %}

DOSCAR\_labels: {% for item in DOSCAR\_labels %}
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{% endfor %}

DOSCAR\_lm\_labels: {% for item in DOSCAR\_lm\_labels %}
- {{ item }}
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EIGENVAL\_title: {{ EIGENVAL\_title }}

EIGENVAL\_n: {{ EIGENVAL\_n }}

EIGENVAL\_nk: {{ EIGENVAL\_nk }}

EIGENVAL\_nLevels: {{ EIGENVAL\_nLevels }}

EIGENVAL\_EList: {% for item in EIGENVAL\_EList %}
- {{ item }}
{% endfor %}

EIGENVAL\_EList\_scf: {% for item in EIGENVAL\_EList\_scf %}
- {{ item }}
{% endfor %}

EIGENVAL\_EList\_all: {% for item in EIGENVAL\_EList\_all %}
- {{ item }}
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InitialStructure\_a: {{ InitialStructure\_a }}

InitialStructure\_b: {{ InitialStructure\_b }}

InitialStructure\_c: {{ InitialStructure\_c }}

InitialStructure\_alpha: {{ InitialStructure\_alpha }}

InitialStructure\_beta: {{ InitialStructure\_beta }}

InitialStructure\_gamma: {{ InitialStructure\_gamma }}

RelaxedStructure\_a: {{ RelaxedStructure\_a }}

RelaxedStructure\_b: {{ RelaxedStructure\_b }}

RelaxedStructure\_c: {{ RelaxedStructure\_c }}

RelaxedStructure\_alpha: {{ RelaxedStructure\_alpha }}

RelaxedStructure\_beta: {{ RelaxedStructure\_beta }}

RelaxedStructure\_gamma: {{ RelaxedStructure\_gamma }}

EIGENVAL\_EV: {{ EIGENVAL\_EV }}

EIGENVAL\_EC: {{ EIGENVAL\_EC }}

EIGENVAL\_Eg: {{ EIGENVAL\_Eg }}