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MedeA VASP Training Session: Explore the comprehensible and user-friendly GUI in *MedeA VASP*

David Reith, Ph.D.
Materials Design

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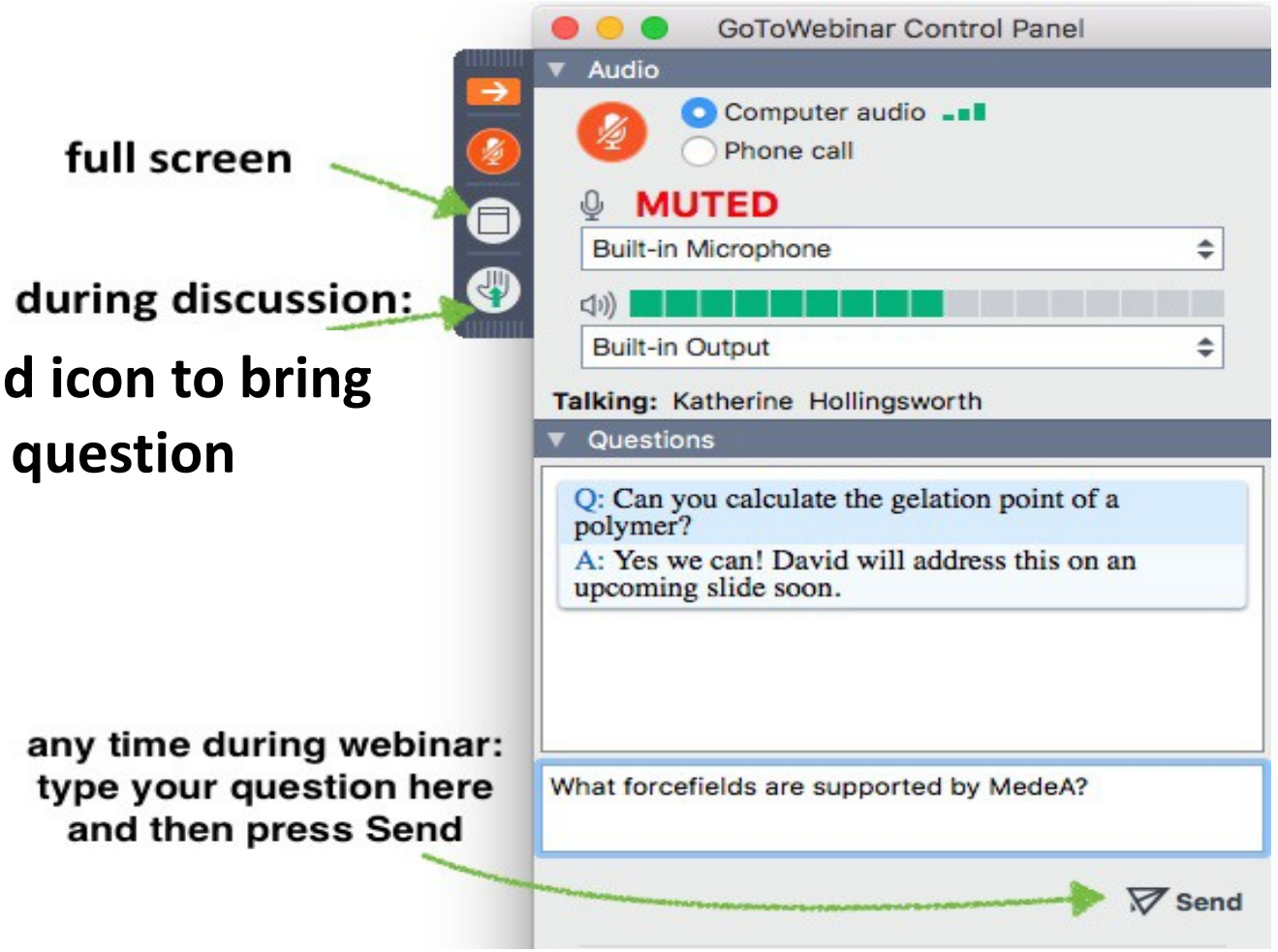

Use the raise hand icon to bring attention to your question

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MedeA VASP Training Session: Explore the comprehensible and user-friendly GUI in *MedeA VASP*

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Outline

- *MedeA VASP*: Overview and General Guidelines
- Heats of Formation: PBE, SCAN and ACFDT-RPA
- Electron Phonon Coupling: Band Gap as a Function of Temperature
- Optical Properties: Color of Materials
- Conclusions

MedeA VASP: Overview

Methods in *MedeA VASP*

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- **DFT**
  - **LDA**
  - GGA-AM05
  - **GGA-PBEsol**
  - **GGA-PBE**
  - **GGA-rPBE**
  - GGA-BLYP
- **Van der Waals DFT**
  - **optB86b-vdW**
  - optB88-vdW
  - optPBE-vdW
  - BEEF-vdW
  - rev-vdW-DF2
  - rPW86-vdW2
  - revPBE-vdW
  - SCAN + rVV10
- **Meta GGA**
  - **revTPSS**
  - TPSS
  - **SCAN**
  - MS2
  - MS1
  - MS0
  - M06-L
  - **MBJLDA**
- **Hybrid Functionals**
  - **HSE06**
  - **PBE0**
  - B3LYP
  - DDH/DSH
- **Screened Exchange**
- **Hartree-Fock**
- **Time dependent DFT**
  - Model Bethe-Salpeter (Excitonic effects)
- **GW/ low scaling GW**
  - **Quasiparticle shifts**
  - Excitonic effects (Bethe-Salpeter)
  - Frequency dependent self-energy
- **MP2**
- **RPA/ low scaling RPA**

Van der Waals correction:

- DFT-D3 zero-damping
- DFT-D3 BJ-damping
- Tkatchenko-Scheffler
- Tkatchenko-Scheffler + SCS
- Many-body dispersion energy
- DFT-dDsC dispersion correction
- DFT-D2 forcefield (Grimme)

LDA+U/GGA+U

- Simplified LSDA+U
- Rotational invariant LSDA+U
- Rotational invariant LDA+U

How to Choose: Optimum Method

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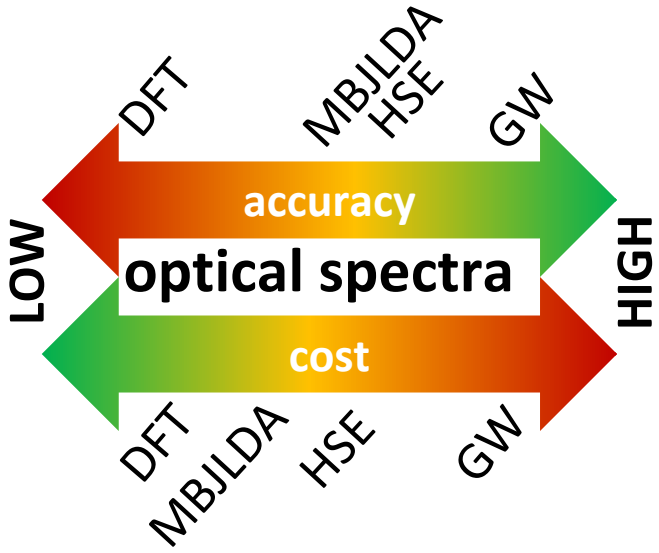
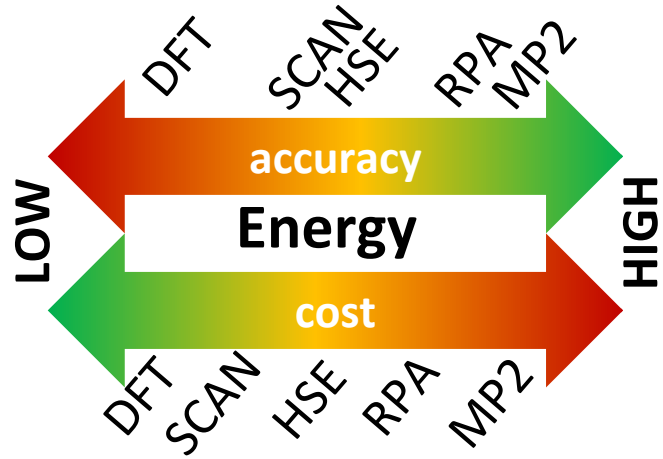
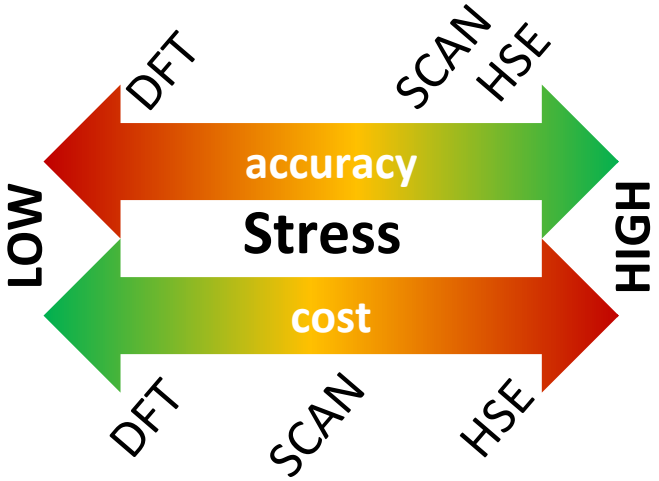
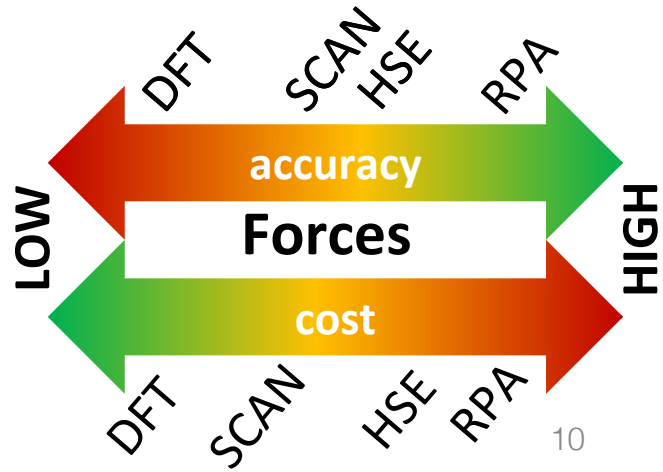
- How accurate does the method need to be for your property?
- Accuracy of method
  vs.
  Applicability for many k-points/ larger systems
- Don't deviate too much from the well-trodden path
  - DFT: LDA, PBE, PBEsol
  - Hybrid: HSE06, PBE0
  - meta-GGA: SCAN, MBJLDA revTPSS
- Only electronic structure: GW, MBJLDA
- Energies: RPA, HSE, SCAN, DFT ..
- Forces: low scaling RPA, SCAN, HSE, DFT
- Stress: HSE, SCAN, DFT









Heat of Formation of SiC

Procedure

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1. Retrieve SiC (F-43m)
2. PBE DFT functional:
    1. Optimize structure
    2. Calculate the heat of formation
3. SCAN meta-GGA functional
    1. Optimize structure
    2. Calculate the heat of formation

How to Choose: k-points and Planewave Cutoff Energies

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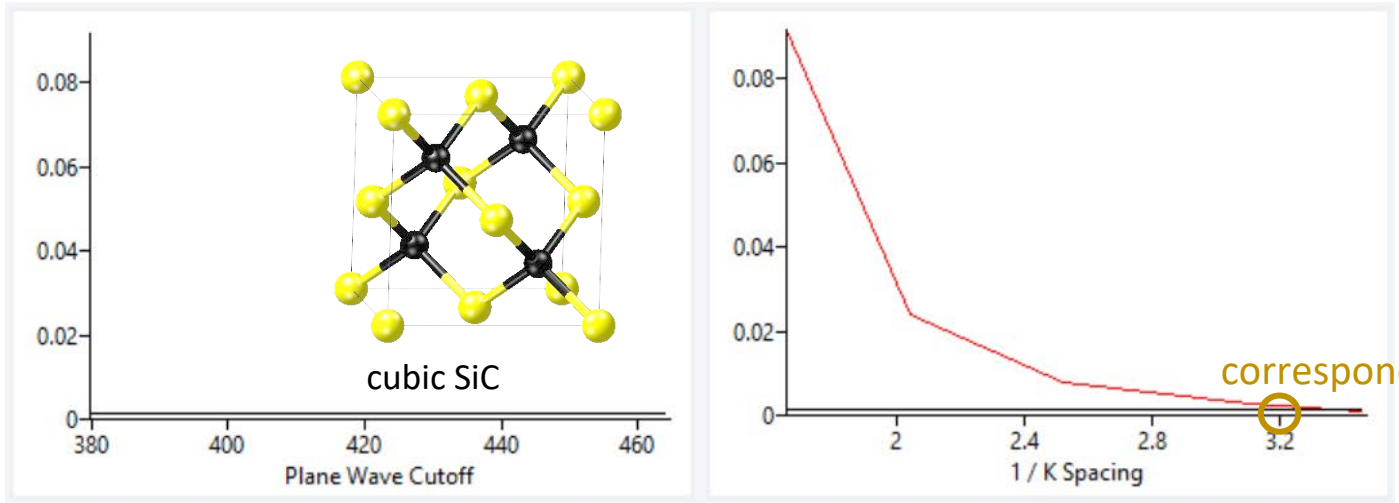
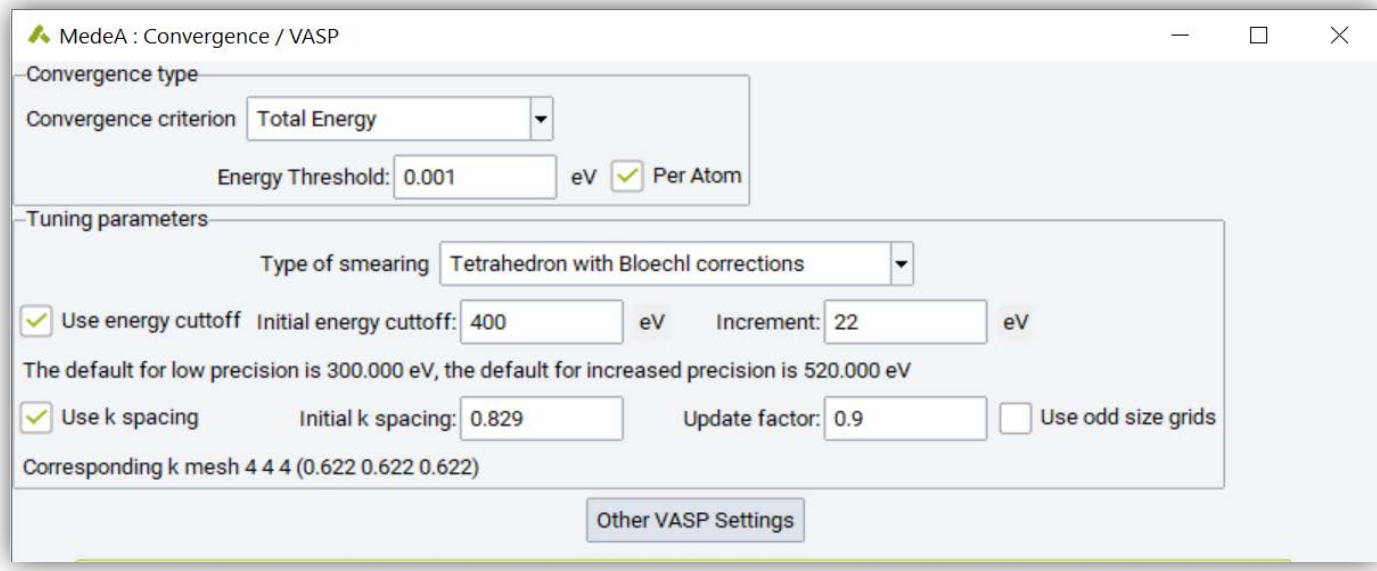


corresponds to 0.3125 1/Ang.

```
-------------------------------------------------------
                The final, converged parameters
-------------------------------------------------------
    Planewave cutoff:  422.000 eV
           k spacing:    0.289 1/Ang

-------------------------------------------------------
               Results for the converged calculation
-------------------------------------------------------
```

- Check convergence of the property that you are interested in
- Always compare like with like:
  - Same k-spacing
  - Same planewave cutoff energy
  - Same integration scheme/smearing width
  - Same method/functional/potentials



Procedure

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1. Retrieve SiC (F-43m)
2. PBE DFT functional:

1. Optimize structure

Calculation tab
Type of calculation Structure Optimization
✔ Relax atom pos. ✔ Allow cell volume to change ✔ Allow cell shape to change
Precision: Standard 500

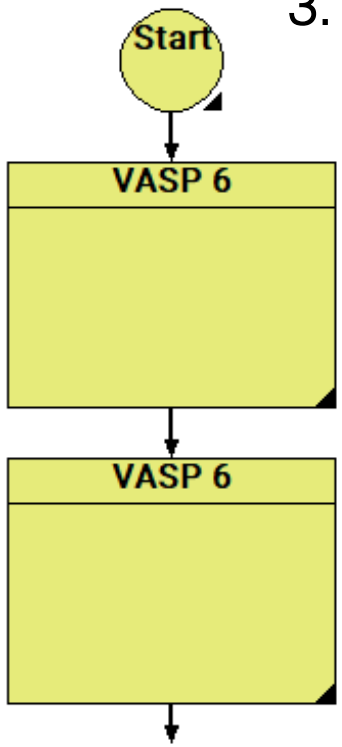
SCF tab
Spacing of k-points: 0.3 **1/Ang.**
Type of smearing Gaussian

2. Calculate the heat of formation

Calculation tab
Type of calculation Single Point
✔ Energy of formation
Precision: Standard 500

SCF tab
Spacing of k-points: 0.3 **1/Ang.**
Type of smearing Gaussian

Procedure



3. Meta-GGA SCAN functional:

1. Optimize structure

Calculation tab
Type of calculation Structure Optimization
✔ Relax atom pos. ✔ Allow cell volume to change
✔ Allow cell shape to change
Functional Meta-GGA, **Type of meta-GGA** SCAN
Precision: Standard 500

SCF tab
Spacing of k-points: 0.3 **1/Ang.**
Type of smearing Gaussian
Maximum iterations: 200
Initial delay of SCF: 10

Advanced/Restart tab
Algorithm Damped molecular dynamics
Number of bands: 12

2. Calculate the heat of formation

Calculation tab
Type of calculation Single Point
✔ Energy of formation
Functional Meta-GGA, **Type of meta-GGA** SCAN
Precision: Standard 500

SCF tab
Spacing of k-points: 0.3 **1/Ang.**
Type of smearing Gaussian

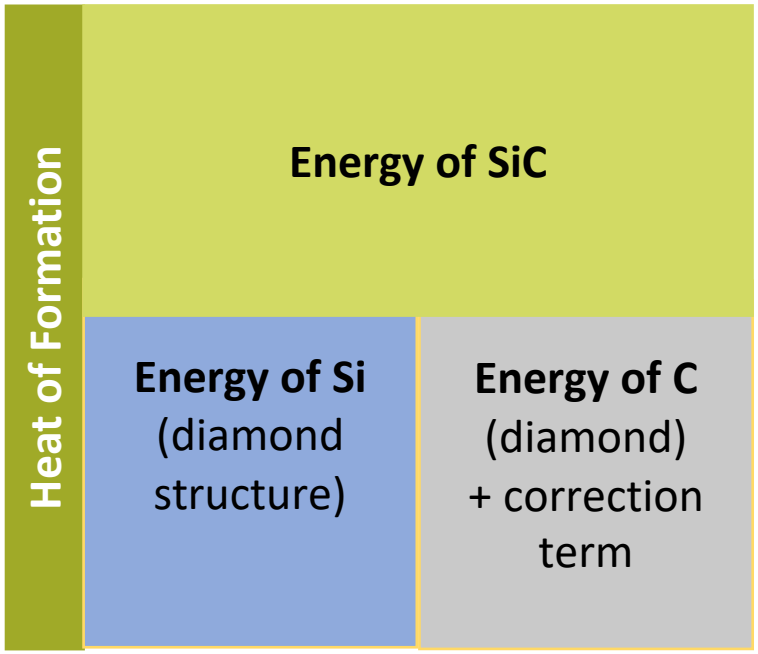
Advanced/Restart tab
Algorithm Damped molecular dynamics
Number of bands: 12

Results

- Use the JobServer web-interface to get results from the relevant **Job.out** files

$$\Delta H_f = E_{SiC} - E_{Si} - E_C$$

Automated Calculation Protocol




```
Details for SiC:
                                                  VASP energy (Etot):    -1453.14 kJ/mol
      Standard state energy of 1.00 atoms of  C  1.00 * -879.23:  -  -879.23
      Standard state energy of 1.00 atoms of Si  1.00 * -523.41:  -  -523.41
                                                                  ----------
                                          Energy of formation (Ef):      -50.50 kJ/mol
```

```
  Details for SiC:
                                                  VASP energy (Etot):    -1998.17 kJ/mol
      Standard state energy of 1.00 atoms of  C  1.00 * -967.94:  -  -967.94
      Standard state energy of 1.00 atoms of Si  1.00 * -966.35:  -  -966.35
                                                                  ----------
                                          Energy of formation (Ef):      -63.88 kJ/mol
```

	PBE (kJ/mol)	SCAN (kJ/mol)	EXP (kJ/mol)
SiC	51	64	**69**

Obtain Accurate Heat of Formation for SiC with ACFDT-RPA

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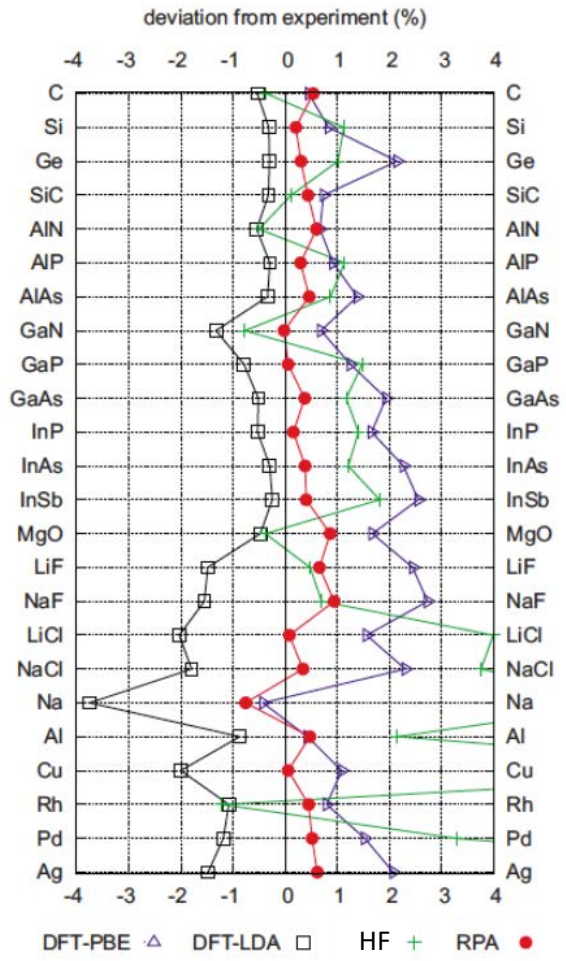
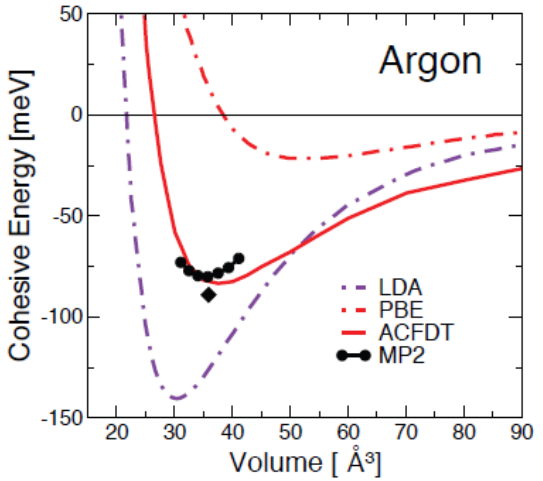
Lattice parameters

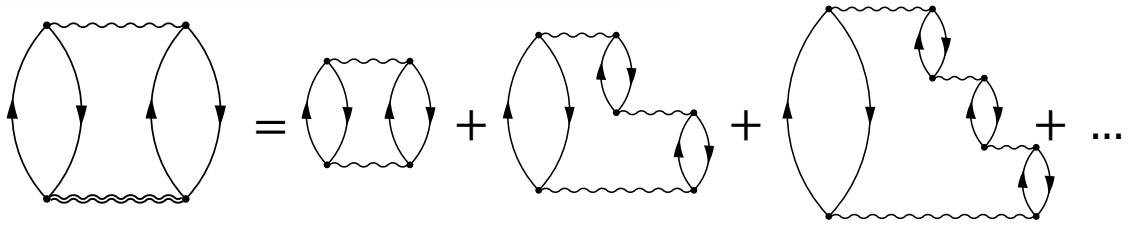


Heats of formation

	PBE	RPA	EXP
LiF	570	609	621
NaF	522	567	576
NaCl	355	405	413
MgO	516	577	603
MgH_2	52	72	78
AlN	262	291	321
SiC	51	**64**	**69**

Van der Waals interactions





2nd. order 3rd. order 4th. order

Introduction

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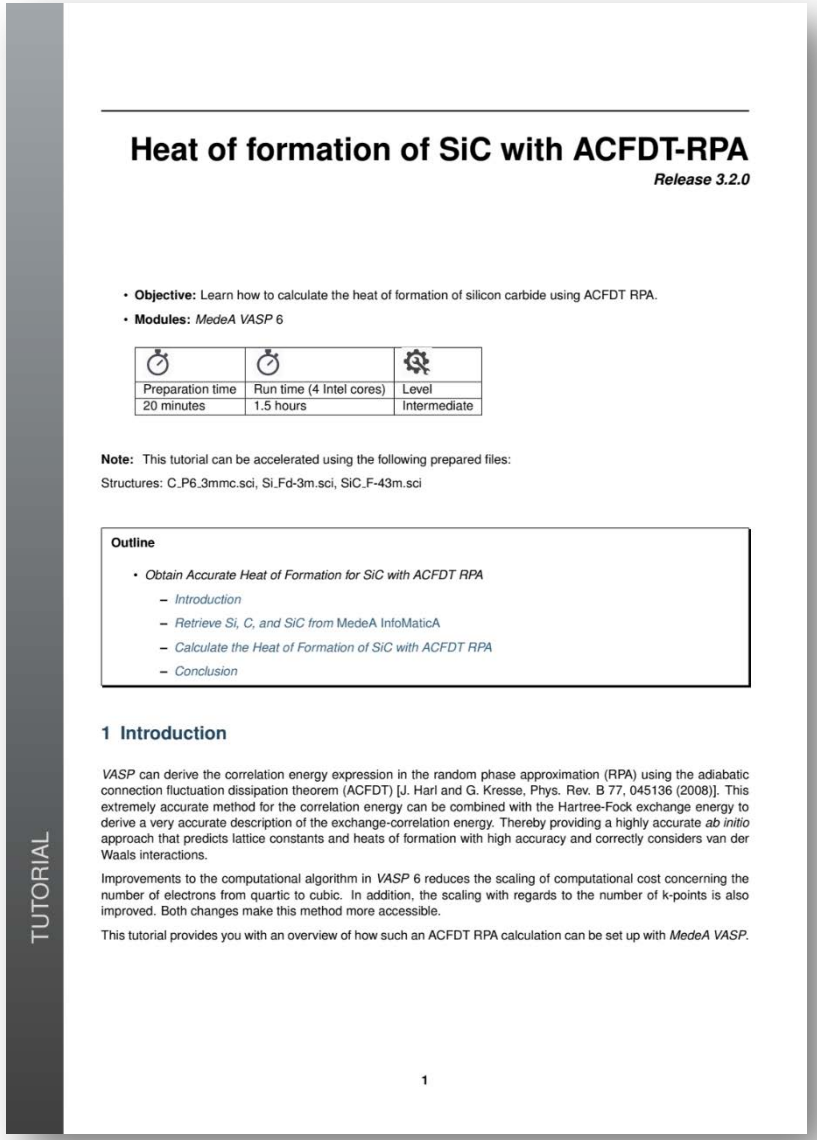
- See *MedeA* tutorial Heat of formation of SiC with ACFDT-RPA at http://my.materialsdesign.com/tutorials

- **Objective:** Learn how to calculate the heat of formation of silicon carbide using ACFDT-RPA.

- **Modules:** *MedeA VASP 6*

Preparation time	Run time (4 Intel cores)	Level
20 minutes	1.5 hours	Intermediate



TUTORIAL

Heat of formation of SiC with ACFDT-RPA

Release 3.2.0

- **Objective:** Learn how to calculate the heat of formation of silicon carbide using ACFDT RPA.
- **Modules:** *MedeA VASP* 6

Preparation time	Run time (4 Intel cores)	Level
20 minutes	1.5 hours	Intermediate

Note: This tutorial can be accelerated using the following prepared files:

Structures: C_P6_3mmc.sci, Si_Fd-3m.sci, SiC_F-43m.sci

Outline

- *Obtain Accurate Heat of Formation for SiC with ACFDT RPA*
  - *Introduction*
  - *Retrieve Si, C, and SiC from* MedeA InfoMaticA
  - *Calculate the Heat of Formation of SiC with ACFDT RPA*
  - *Conclusion*

1 Introduction

VASP can derive the correlation energy expression in the random phase approximation (RPA) using the adiabatic connection fluctuation dissipation theorem (ACFDT) [J. Harl and G. Kresse, Phys. Rev. B 77, 045136 (2008)]. This extremely accurate method for the correlation energy can be combined with the Hartree-Fock exchange energy to derive a very accurate description of the exchange-correlation energy. Thereby providing a highly accurate *ab initio* approach that predicts lattice constants and heats of formation with high accuracy and correctly considers van der Waals interactions.

Improvements to the computational algorithm in *VASP* 6 reduces the scaling of computational cost concerning the number of electrons from quartic to cubic. In addition, the scaling with regards to the number of k-points is also improved. Both changes make this method more accessible.

This tutorial provides you with an overview of how such an ACFDT RPA calculation can be set up with *MedeA VASP*.

1

Procedure

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1. Retrieve SiC (F-43m), Si (Fd-3m) and C (P6_3/mmc)
2. Define and run the ACFDT-RPA calculation
3. Calculate the heat of formation from ACFDT-RPA total energies

Results

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- Use the JobServer web-interface to open the relevant **Job.out**

```
 ACFDT-RPA correlation energy:             -12.219715 eV for Si2
      Hartree-Fock total energy:             -18.509282 eV for Si2
Correction for partial occupancy:              -0.000000 eV for Si2
------------------------------------------------------------------
          ACFDT-RPA total energy:             -30.728997 eV for Si2

Electronic contributions:
                          Empirical Formula          Cell
                                      Si            (Si)8
                          --------------- ---------------
         ACFDT-RPA Energy       -1482.448      -11859.587 kJ/mol
```

```
 ACFDT-RPA correlation energy:             -27.349385 eV for C4
      Hartree-Fock total energy:             -61.141280 eV for C4
Correction for partial occupancy:              -0.000000 eV for C4
------------------------------------------------------------------
          ACFDT-RPA total energy:             -88.490665 eV for C4

Electronic contributions:
                          Empirical Formula          Cell
                                      C             (C)4
                          --------------- ---------------
         ACFDT-RPA Energy       -2134.512       -8538.049 kJ/mol
```

```
 ACFDT-RPA correlation energy:             -13.011143 eV for SiC
      Hartree-Fock total energy:             -25.144840 eV for SiC
Correction for partial occupancy:              -0.000000 eV for SiC
------------------------------------------------------------------
          ACFDT-RPA total energy:             -38.155983 eV for SiC

Electronic contributions:
                          Empirical Formula          Cell
                                     SiC            (SiC)4
                          --------------- ---------------
         ACFDT-RPA Energy       -3681.492      -14725.967 kJ/mol
```

	PBE (kJ/mol)	SCAN (kJ/mol)	RPA (kJ/mol)	EXP (kJ/mol)
SiC	51	64	65	**69**

graphite as reference

$$\Delta H_f = E_{SiC} - E_{Si} - E_C = -3681.492+1482.448+2134.512=\mathbf{-64.53}\ \text{kJ/mol}$$

ACFDT-RPA: Computational Cost

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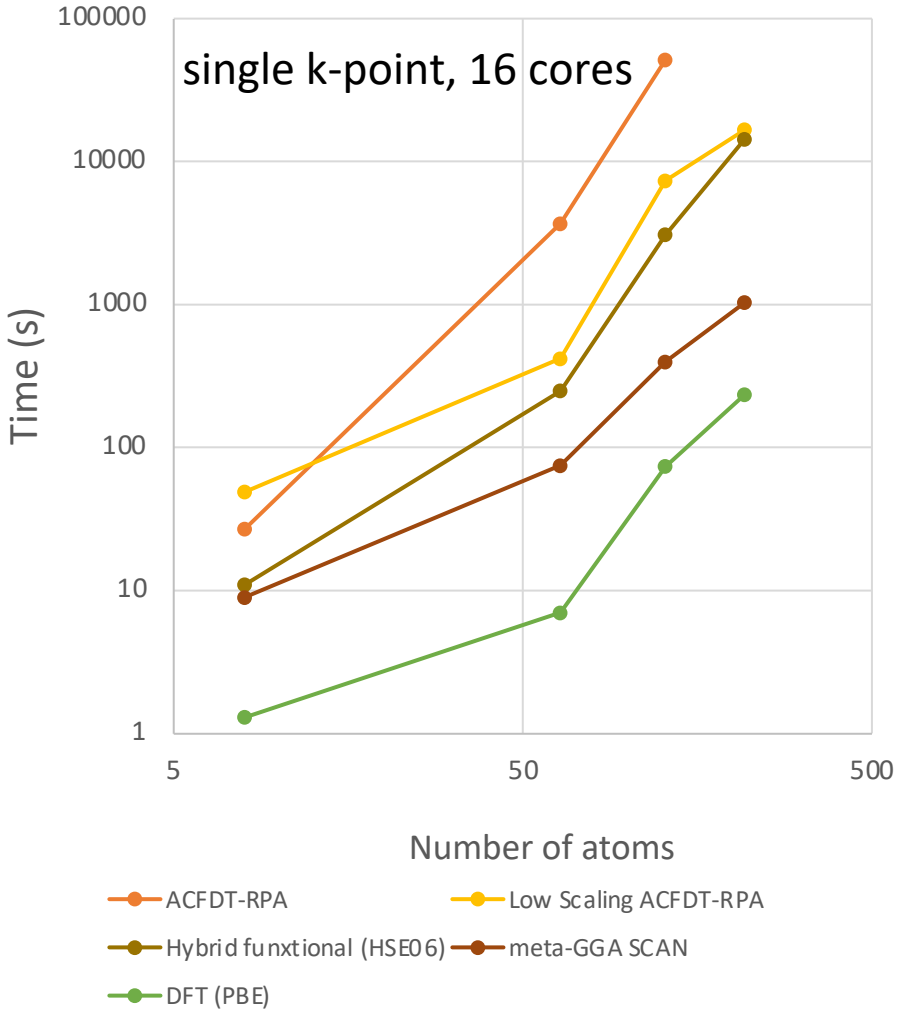

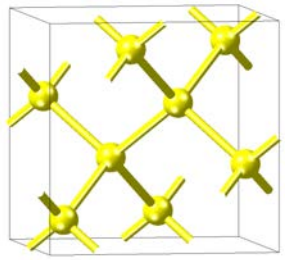

silicon

ACFDT-RPA: Computational Cost

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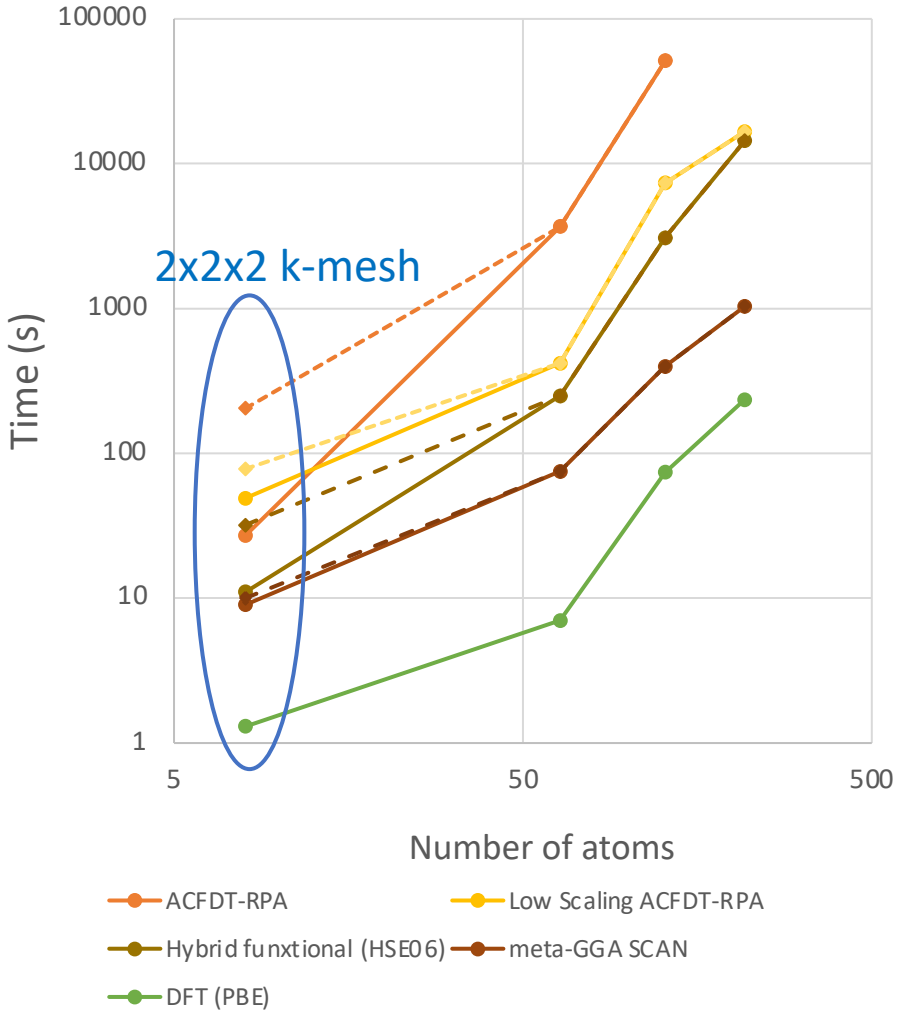
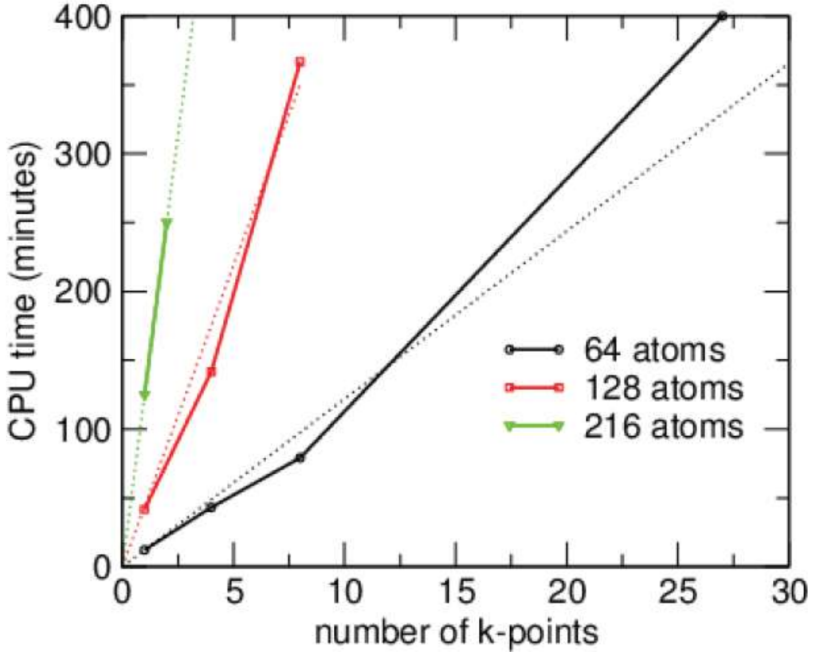
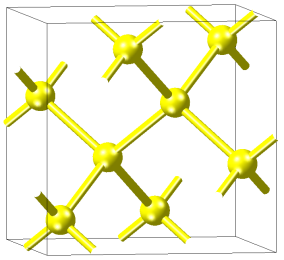


Scaling of low scaling RPA with k-points:





silicon

Conclusion

- Tutorial showed how to calculate the heat of formation using PBE, SCAN, and ACFDT RPA
- Calculated silicon carbide HoF is 64.5 kJ/mol

- See also:

  The Random Phase Approximation: A Practical Method Beyond DFT
  https://my.materialsdesign.com/webinar-41

  VASP 6: Total energies beyond DFT
  https://my.materialsdesign.com/webinar-35

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Interlude

MedeA VASP: Handling of Symmetry in Structures

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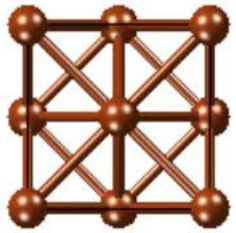
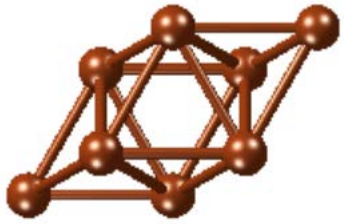
Cu (Fm-3m)



Atoms

Atom	Name	Element	Atomic Number	Wyckoff Position	Wyckoff Equation
1	Cu1	Cu	29	4a	0,0,0



Structure used in VASP with full consideration of symmetry

- Definition of high symmetry points in 1st Brillouin zone for band structures
- DFT calculation structure contains a single atom instead of 4 atoms
- Use of symmetry to reduce calculation effort
- Etc.

MedeA VASP: Handling of Symmetry in Structures

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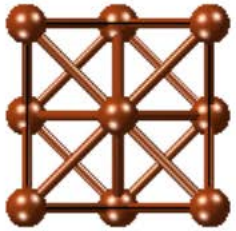
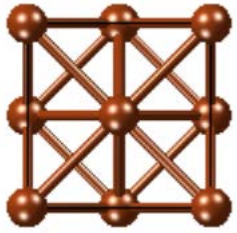
Cu (P1)



Atoms

Atom	Name	Element	Atomic Number	Wyckoff Position	Wyckoff Equation
1	Cu1	Cu	29	1a	x,y,z
2	Cu2	Cu	29	1a	x,y,z
3	Cu3	Cu	29	1a	x,y,z
4	Cu4	Cu	29	1a	x,y,z



Structure used in VASP without consideration of symmetry

- Definition of high symmetry points in 1st Brillouin zone based on P1 symmetry
- Instead of 1 Cu atom structure contains 4 Cu atoms → increase in calculation effo
- In most cases no use of symmetry to reduce calculation effort (MT, Phonon, etc.) (VASP still uses symmetry – can be switched off in the Advanced/Restart tab)

MedeA VASP: Sites vs. Atom Positions

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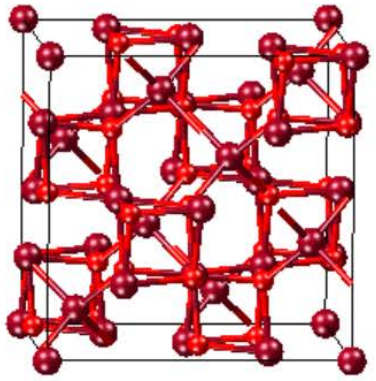
- With symmetry: **sites ≠ atom positions**



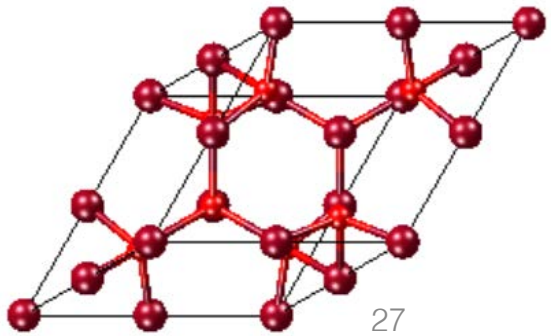
Fe_3O_4 (Fd-3m)

Atoms

Atom	Name	Element	Atomic Number	Wyckoff Position	Wyckoff Equation	X
1	O	O	8	32e	x,x,x	0.2297
2	Fe1	Fe	26	16c	0,0,0	0
3	Fe2	Fe	26	8b	3/8,3/8,3/8	0.375

POSCAR:

```
(Fe3O4)8   (Fd-3m) ~ (Pearson #1221350)_1 (VASP)
    1.0
            0.00000000 4.19650000 4.19650000
            4.19650000 0.00000000 4.19650000
            4.19650000 4.19650000 0.00000000
  8 6
Direct
        0.22970000 0.22970000 0.22970000
        -0.18910000 0.22970000 0.22970000
        0.22970000 -0.18910000 0.22970000
        0.22970000 0.22970000 -0.18910000
        0.77030000 0.77030000 0.77030000
        0.18910000 0.77030000 0.77030000
        0.77030000 0.18910000 0.77030000
        0.77030000 0.77030000 0.18910000
        0.00000000 0.00000000 0.00000000
        0.50000000 0.00000000 0.00000000
        …
```



MedeA VASP: Sites vs. Atom Positions

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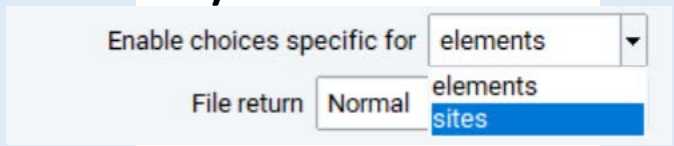
Atoms — Fe_3O_4 (Fd-3m)

Atom	Name	Element	Atomic Number	Wyckoff Position	Wyckoff Equation	X
1	O	O	8	32e	x,x,x	0.2297
2	Fe1	Fe	26	16c	0,0,0	0
3	Fe2	Fe	26	8b	3/8,3/8,3/8	0.375

POSCAR:

```
(Fe3O4)8  (Fd-3m) ~ (Pearson #1221350)_1 (VASP)
    1.0
          0.00000000 4.19650000 4.19650000
          4.19650000 0.00000000 4.19650000
          4.19650000 4.19650000 0.00000000
  8 6
Direct
        0.22970000 0.22970000 0.22970000
       -0.18910000 0.22970000 0.22970000
        0.22970000 -0.18910000 0.22970000
        0.22970000 0.22970000 -0.18910000
        0.77030000 0.77030000 0.77030000
```

Advanced/Restart tab

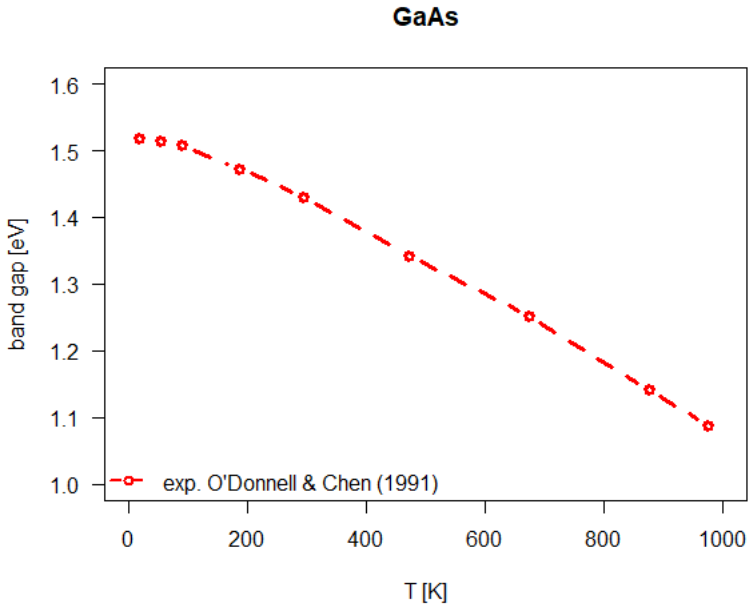


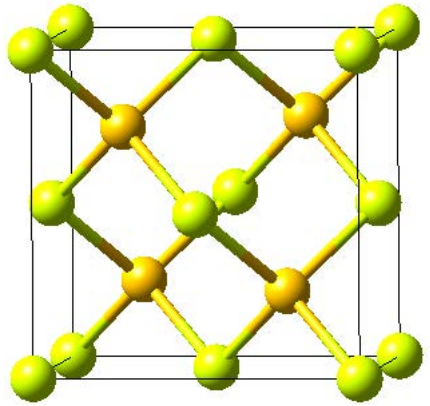
POSCAR:

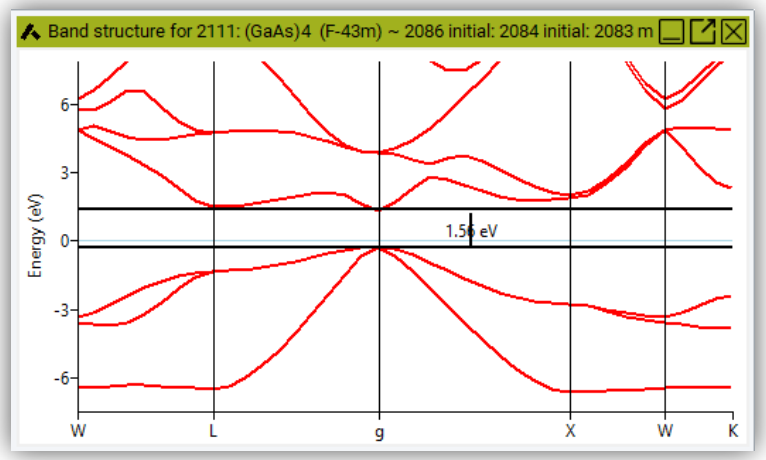
```
(Fe3O4)8  (Fd-3m) ~ (Pearson #1221350)_1 (VASP)
    1.0
          0.00000000 4.19650000 4.19650000
          4.19650000 0.00000000 4.19650000
          4.19650000 4.19650000 0.00000000
  8 4 2
Direct
        0.22970000 0.22970000 0.22970000
       -0.18910000 0.22970000 0.22970000
        0.22970000 -0.18910000 0.22970000
        0.22970000 0.22970000 -0.18910000
        0.77030000 0.77030000 0.77030000
```

- LDA+U/GGA+U: apply different U(&J) values to different sites occupied by the same element
- XANES spectroscopy with MedeA VASP 6: specify a site containing a single atom position

Electron Phonon Coupling: Phonon Induced Change of Band Gap of GaAs as a Function of Temperature







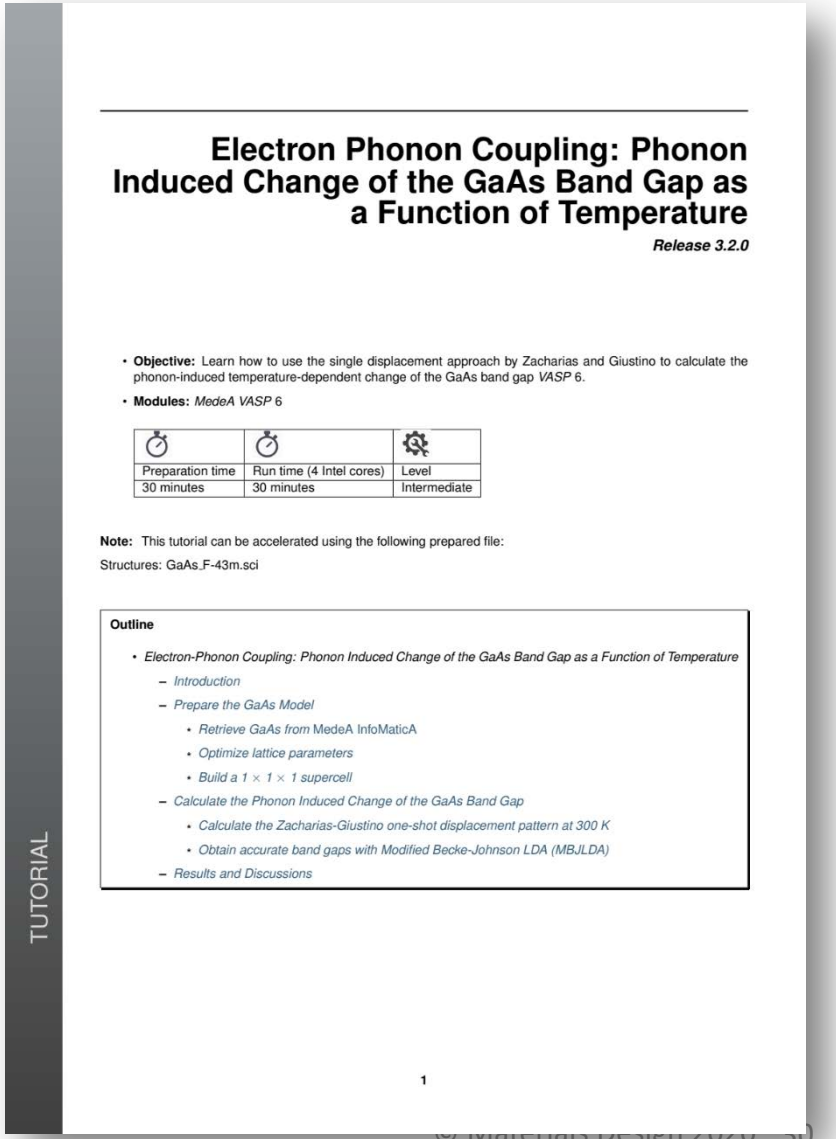
Introduction

- See *MedeA* tutorial Electron Phonon Coupling: Phonon Induced Change of the GaAs Band Gap as a Function of Temperature at http://my.materialsdesign.com/tutorials

- **Objective:** Learn how to use the single displacement approach by Zacharias and Giustino to calculate the phonon-induced temperature-dependent change of the GaAs band gap by *VASP* 6.

- **Modules:** *MedeA VASP 6*

Preparation time	Run time (4 Intel cores)	Level
30 minutes	30 minutes	Intermediate


TUTORIAL

Electron Phonon Coupling: Phonon Induced Change of the GaAs Band Gap as a Function of Temperature

Release 3.2.0

- **Objective:** Learn how to use the single displacement approach by Zacharias and Giustino to calculate the phonon-induced temperature-dependent change of the GaAs band gap *VASP* 6.
- **Modules:** *MedeA VASP* 6

Preparation time	Run time (4 Intel cores)	Level
30 minutes	30 minutes	Intermediate

Note: This tutorial can be accelerated using the following prepared file:
Structures: GaAs_F-43m.sci

Outline

- *Electron-Phonon Coupling: Phonon Induced Change of the GaAs Band Gap as a Function of Temperature*
  - *Introduction*
  - *Prepare the GaAs Model*
    - *Retrieve GaAs from* MedeA InfoMaticA
    - *Optimize lattice parameters*
    - *Build a 1 × 1 × 1 supercell*
  - *Calculate the Phonon Induced Change of the GaAs Band Gap*
    - *Calculate the Zacharias-Giustino one-shot displacement pattern at 300 K*
    - *Obtain accurate band gaps with Modified Becke-Johnson LDA (MBJLDA)*
  - *Results and Discussions*

1

Procedure

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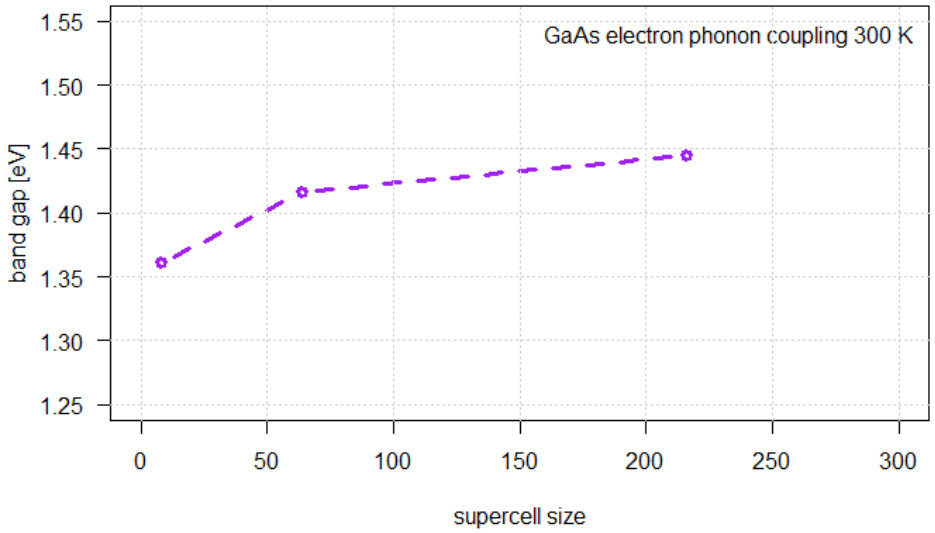
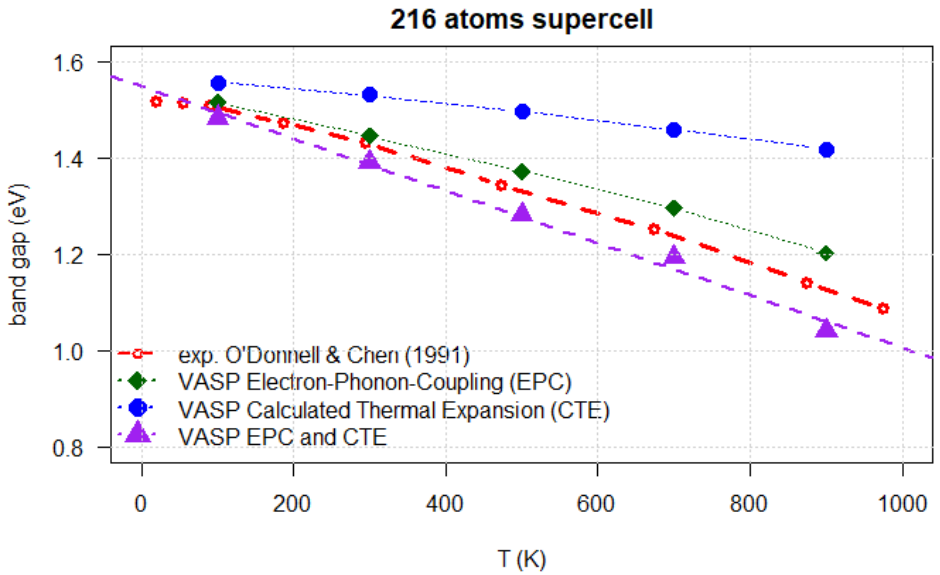
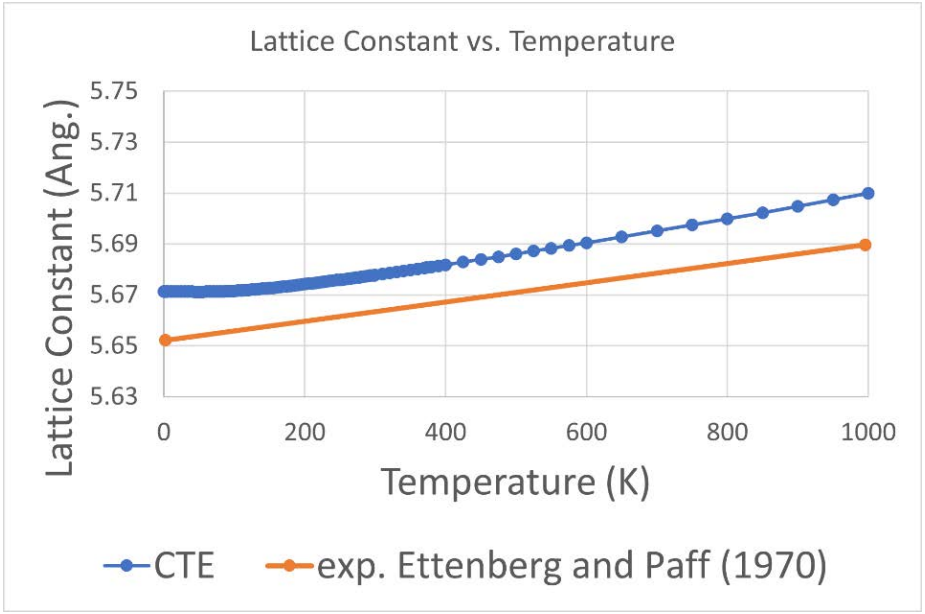
1. Retrieve crystal structure of GaAs
2. Optimize the structure with PBEsol
3. Build a 1x1x1 supercell
4. Calculate the Zacharias-Giustino one-shot displacement pattern at 300 K
5. Obtain accurate band gaps with Modified Becke-Johnson LDA

	Exp.	PBE	PBEsol	LDA
Lattice constant (Ang.)	**5.653**	5.756	**5.662**	5.610

Phonon Induced Temperature Dependent Change of the Band Gap

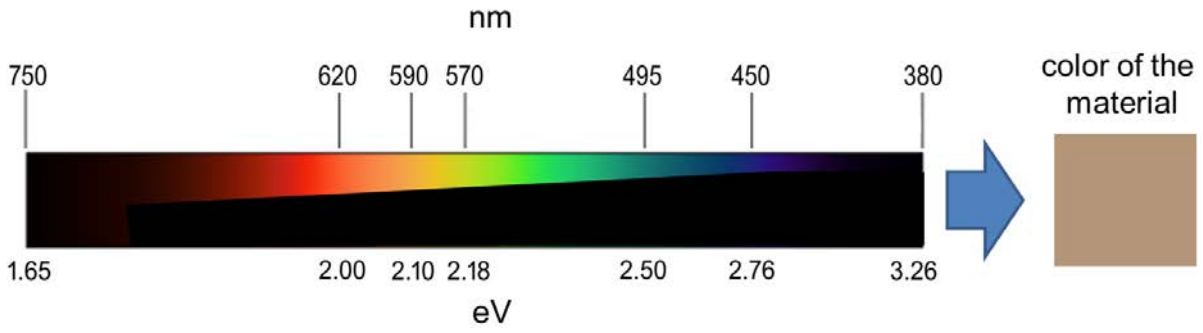


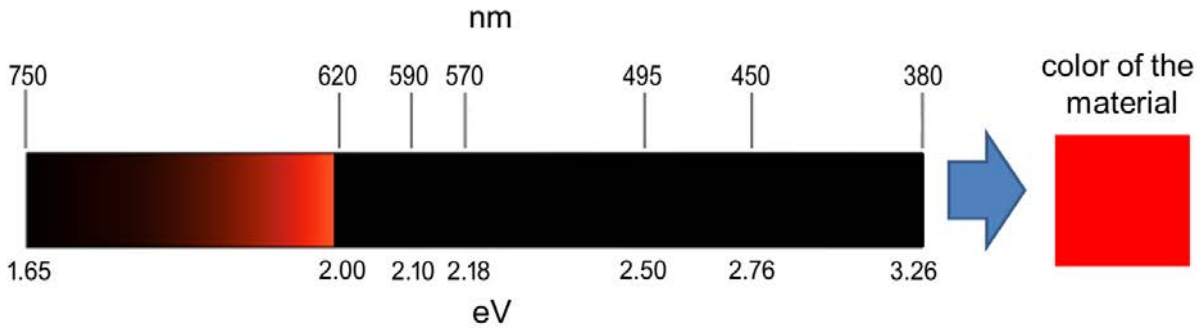


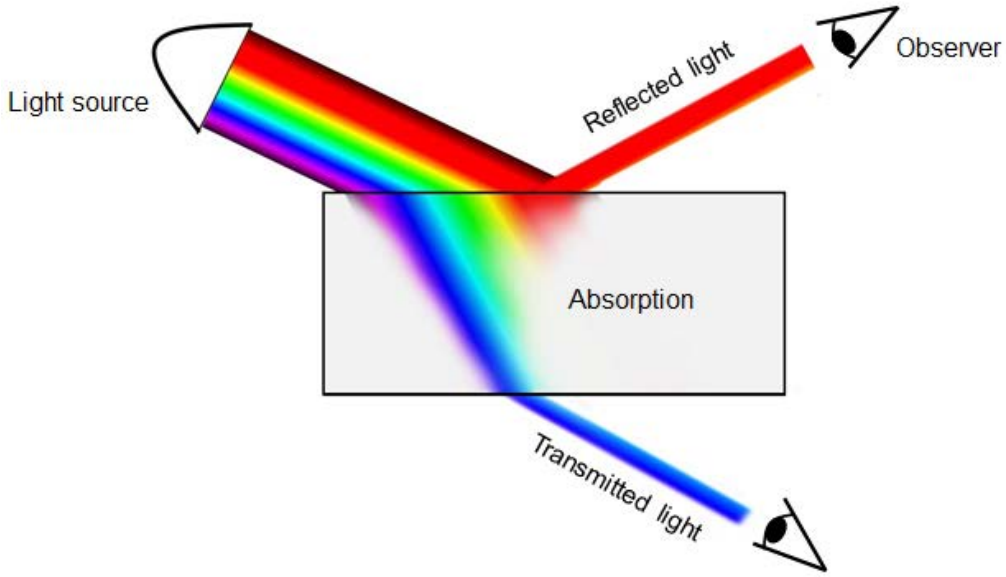


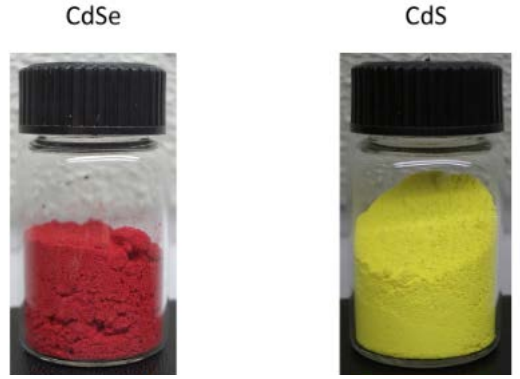
- Need large supercells
- Include thermal expansion to consider all important contributions
- Other properties can also be computed from the single displacement pattern (e.g., optical properties)
- Procedure:
  - Lattice optimization with PBEsol
  - One-shot displacement pattern (Zacharias&Giustino)
  - Band gaps with MBJLDA

Color of Cadmium Selenide and Cadmium Sulfide









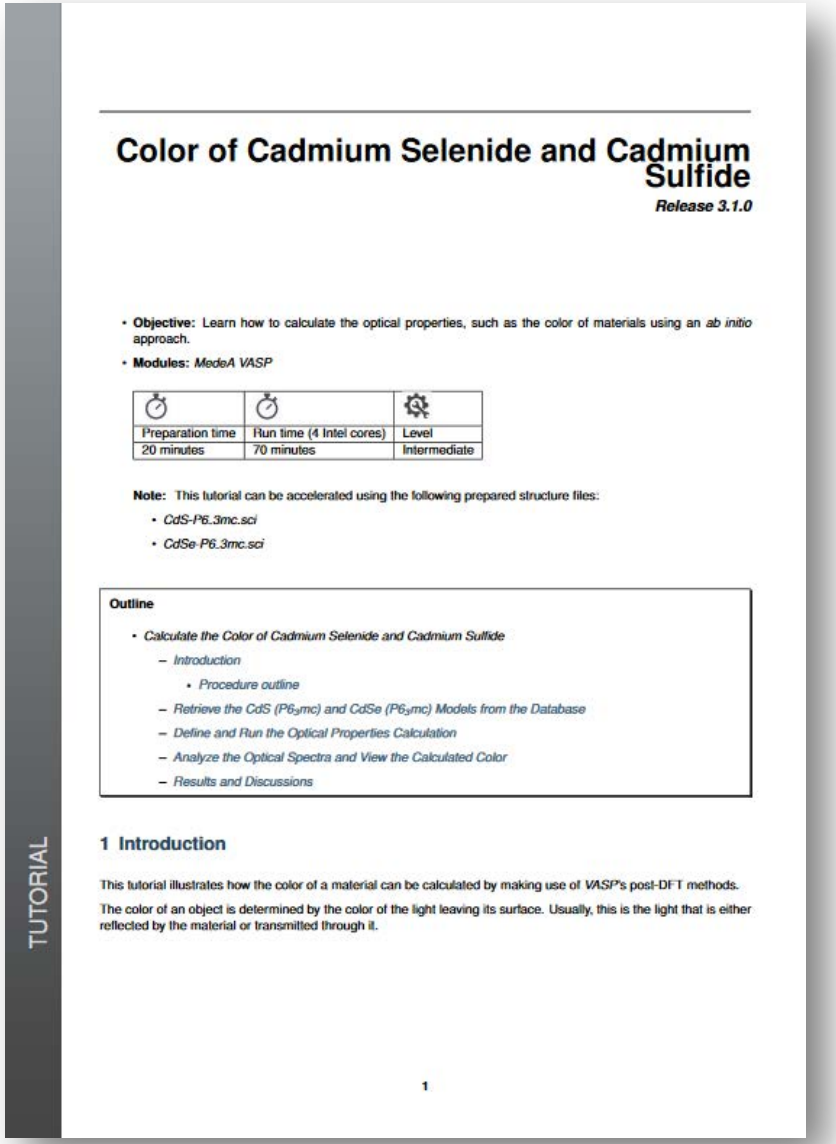
Introduction

- See *MedeA* tutorial Calculate the Color of Cadmium Selenide and Cadmium Sulfide at http://my.materialsdesign.com/tutorials

- **Objective:** Learn how to calculate the optical properties, such as the color of materials using an *ab initio* approach.

- **Modules:** *MedeA VASP*

Preparation time	Run time (4 Intel cores)	Level
20 minutes	70 minutes	Intermediate



TUTORIAL

Color of Cadmium Selenide and Cadmium Sulfide

Release 3.1.0

- **Objective:** Learn how to calculate the optical properties, such as the color of materials using an *ab initio* approach.
- **Modules:** *MedeA VASP*

Preparation time	Run time (4 Intel cores)	Level
20 minutes	70 minutes	Intermediate

Note: This tutorial can be accelerated using the following prepared structure files:

- *CdS-P6_3mc.sci*
- *CdSe-P6_3mc.sci*

Outline

- *Calculate the Color of Cadmium Selenide and Cadmium Sulfide*
  - *Introduction*
    - *Procedure outline*
  - *Retrieve the CdS ($P6_3mc$) and CdSe ($P6_3mc$) Models from the Database*
  - *Define and Run the Optical Properties Calculation*
  - *Analyze the Optical Spectra and View the Calculated Color*
  - *Results and Discussions*

1 Introduction

This tutorial illustrates how the color of a material can be calculated by making use of *VASP*'s post-DFT methods.

The color of an object is determined by the color of the light leaving its surface. Usually, this is the light that is either reflected by the material or transmitted through it.

1

MedeA VASP: Automated Calculation Protocol

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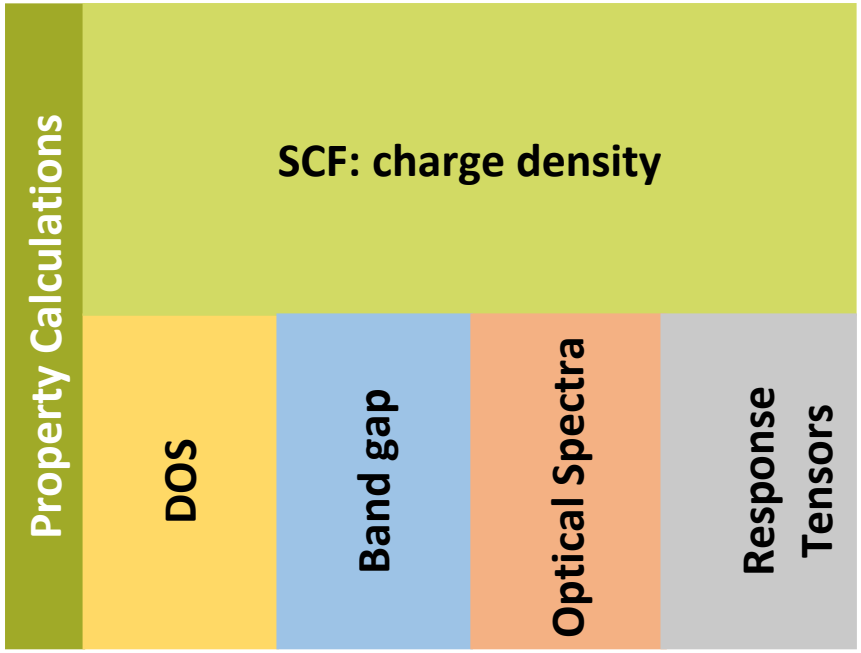
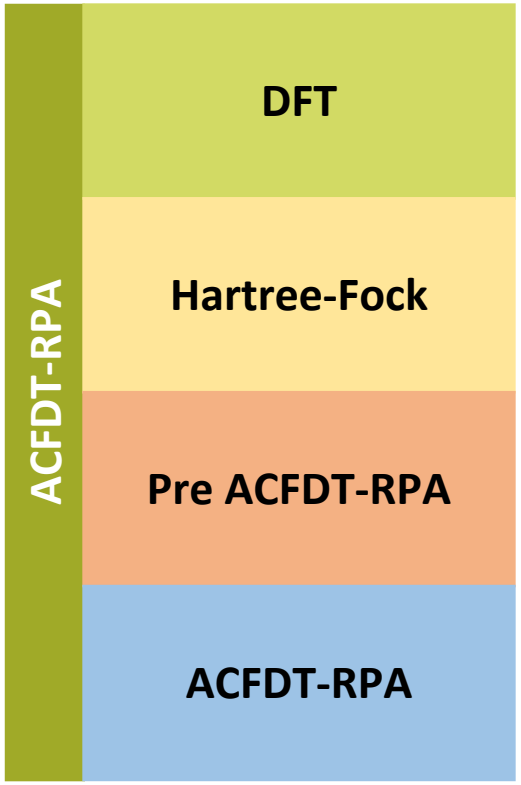
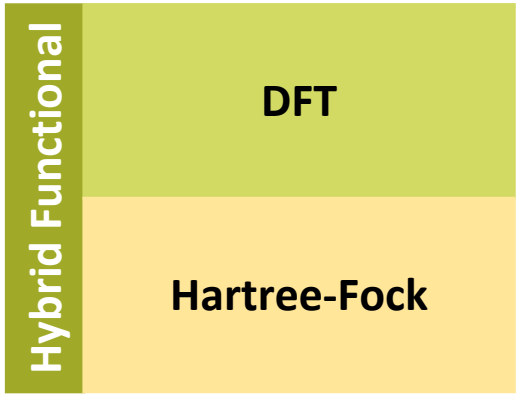




Job.out:

```
VASP 6 CALCULATION PROTOCOL:
============================
1. Single point calculation
     Saved properties in this step: wave  functions
2. Calculate Hartree-Fock energy E_EXX evaluated
   non self-consistently using orbitals from previous step
3. Prepare for ACFDT-RPA by calculation of a large
   number of accurate excited states
4. Calculate the ACFDT-RPA correlation energy
```



...

Procedure Outline

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1. Retrieve crystal structures of CdSe and CdS
2. Optimize these structures with PBE
3. Define and run the optical spectra calculation using MBJLDA
4. Analyze the optical spectra and view the resulting color

Optical Spectra Analysis

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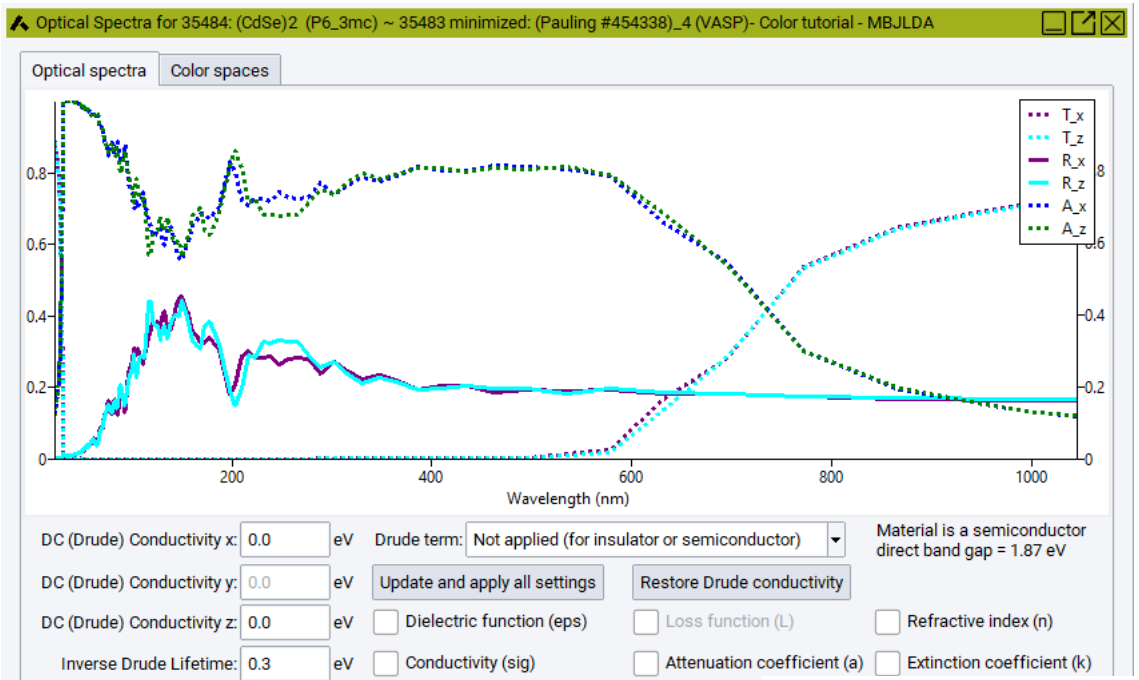
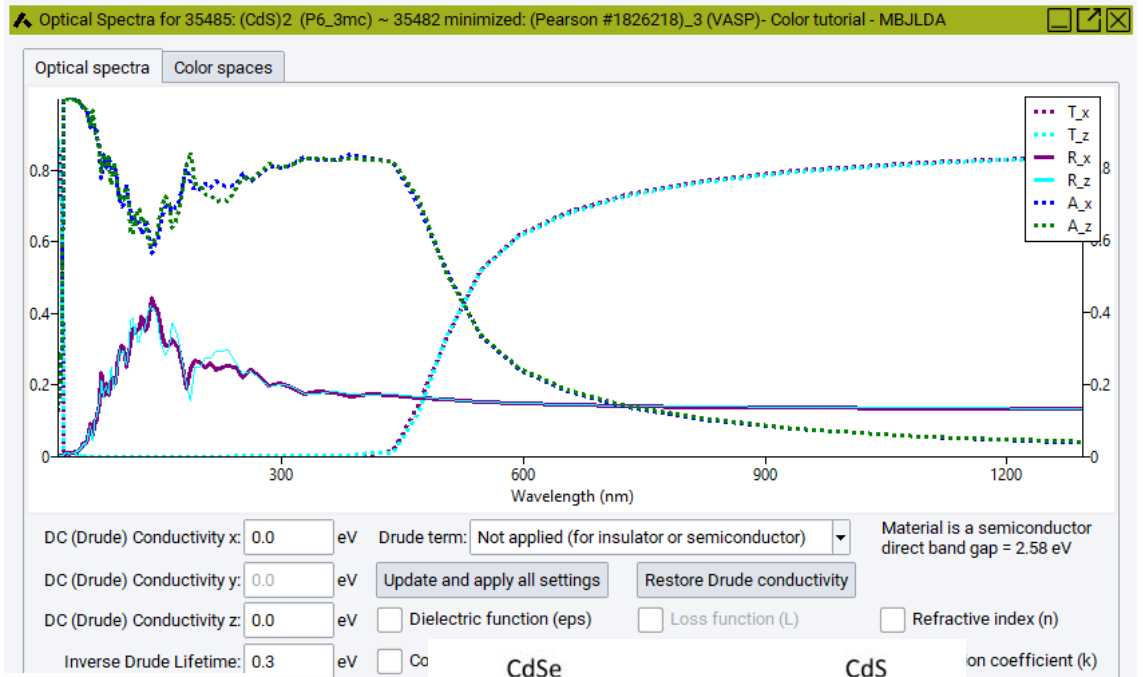
- CdSe

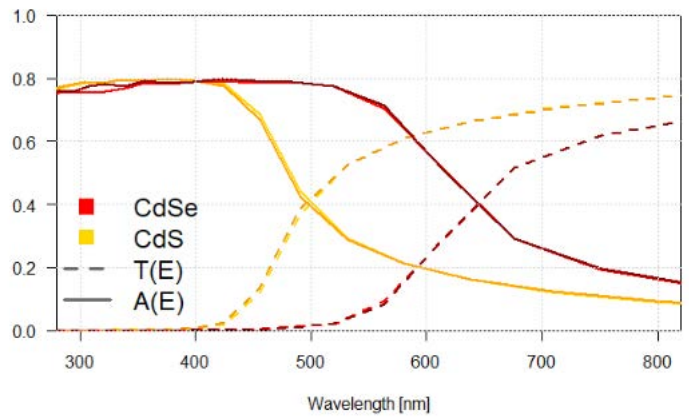


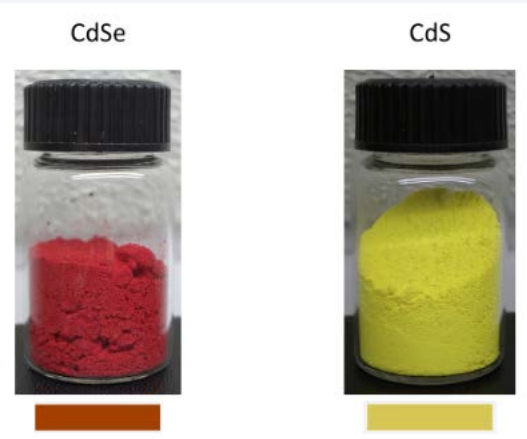
- CdS



	MBJLDA	Exp.
CdSe	1.87 eV	1.74 eV
CdS	2.58 eV	2.42 eV

band gap





Conclusion

- Tutorial showed how to predict the color of CdSe and CdS with MedeA VASP
- Good prediction of the electronic structure → good prediction of the optical spectra → good color prediction
- Modified Becke Johnson LDA predicts the electronic structure well
  - It is computationally much cheaper than other “accurate” methods
  - It yields “accurate” enough electronic structures
  - It can only be used to calculate the electronic structure

- See also:

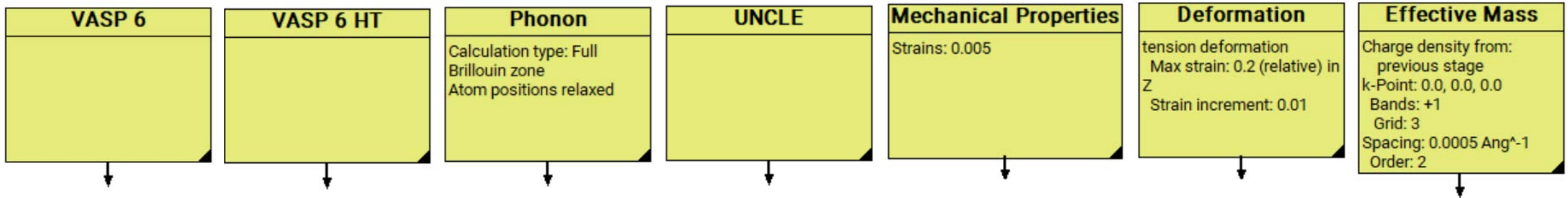
The Color of Materials: Value from Computed Optical Properties
http://my.materialsdesign.com/webinar-25

MedeA VASP

materials design®

- Integrated with other property modules
  - *MedeA Phonon*: Phonon spectra, IR, Raman spectra, thermodynamic functions (vibrational free energy, heat capacities)
  - *MedeA MT*: Elastic, mechanical and thermodynamic properties
  - *MedeA Transition State Search*: Reaction pathways, structure and energy of transition states
  - *MedeA Electronics*: Fermi surfaces, electronic contributions to the electrical and thermal conductivity, thermoelectric power, and effective masses
  - *MedeA UNCLE*: Cluster expansion – search and identify ground states – Monte Carlo simulation to study phase stability
  - *MedeA Forcefield Optimizer*: Optimize forcefield parameters based on VASP ab initio

- *MedeA* Flowcharts: high throughput calculations



MedeA VASP

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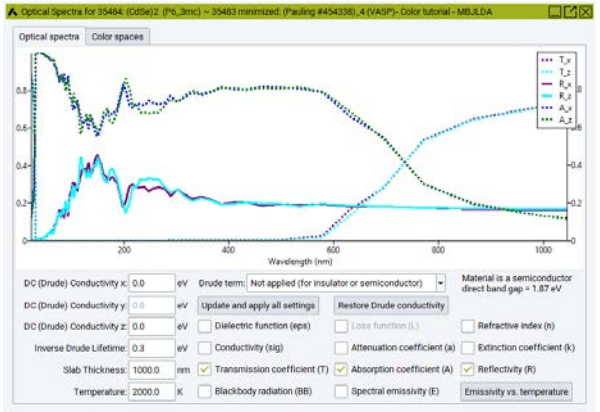
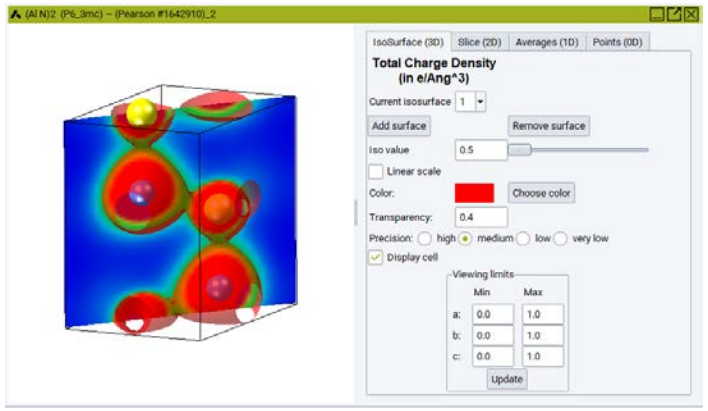
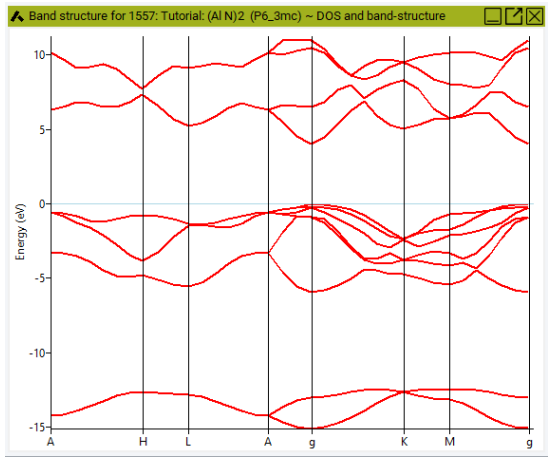
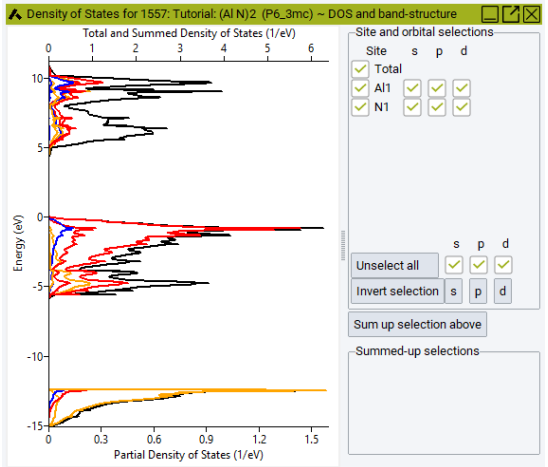
- An easy and straightforward way to set up your calculations
- More than a graphical user interface
  - Make use of the automated VASP calculation protocols
  - Reliably define and run high-throughput calculations with Flowcharts
  - Post-processing to get and summarize the results that you are interested in
  - Analyze results using interactive tools









Upcoming Webinar

Advancing Automotive Innovation with Materials Modeling

www.materialsdesign.com/webinars

April 29th, 2021
7:00 a.m. PDT / 10:00 a.m. EDT / 16:00 CET

VOLKSWAGEN
AKTIENGESELLSCHAFT

Dr. Jonathan Mueller
Senior Scientist,
Volkswagen AG

MedeA Modules Used in the Training

- *MedeA Environment*
- *MedeA InfoMaticA & Databases*
- *MedeA VASP 6*
- Webinar: Live and Recorded
  https://www.materialsdesign.com/webinars
  - Recorded Webinars Recommended During Today's Training

    The Random Phase Approximation: A Practical Method Beyond DFT

    VASP 6: Total energies beyond DFT

    The Color of Materials: Value from Computed Optical Properties

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- Application Notes
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- For questions or comments contact:

Katherine Hollingsworth
khollingsworth@materialsdesign.com

Question and Answer Session

Dr. René Windiks

Materials Design

Dr. David Reith

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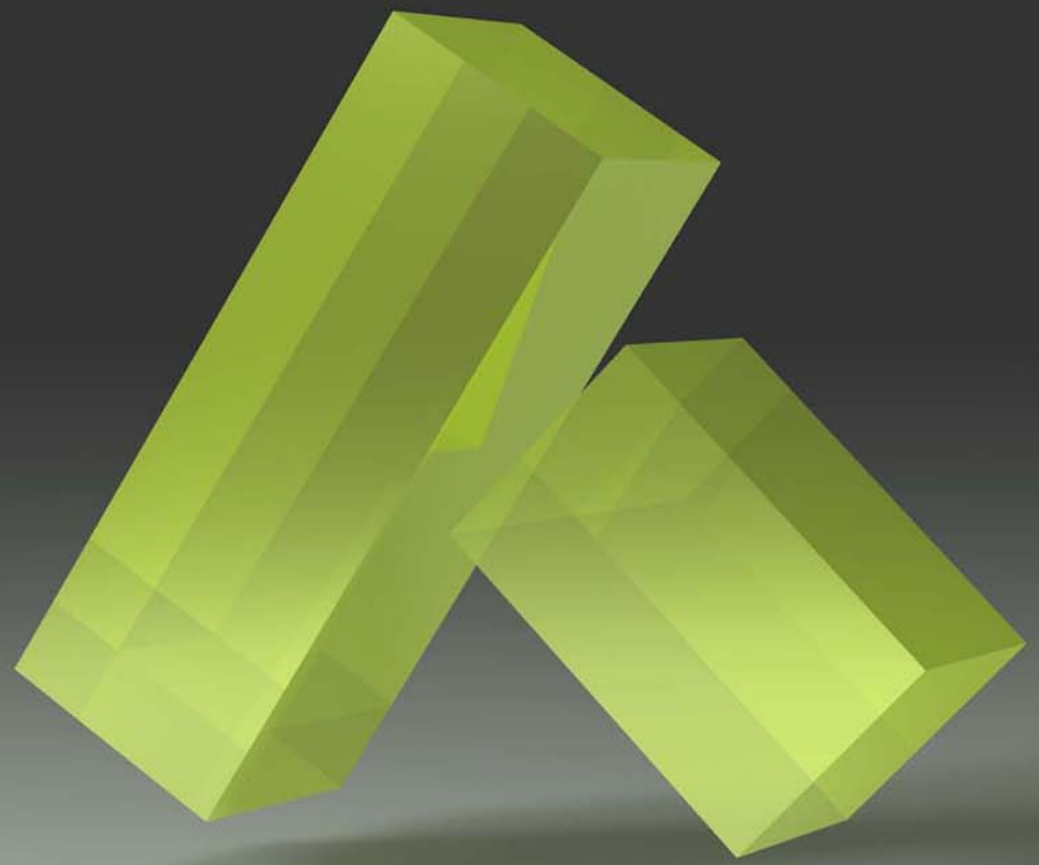

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Innovation by Simulation