

UGM 2020 Training Series

MedeA VASP 6: Random Phase Approximation, Electron-Phonon Coupling, etc.

Materials Design

October 20th, 2020

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Please Ask Questions!







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MedeA VASP 6: Random Phase Approximation, Electron-Phonon Coupling, etc.

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Outline



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

MedeA VASP 6: Overview

Methods in MedeA VASP





How to Choose: Optimum Method

- 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





How to Choose: k-points and Planewave Cutoff Energies





- 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

j			
Convergence criterion	Total Energy		
Ener	gy Threshold: 0.001 eV Per Atom		
Tuning parameters			
	Type of smearing Methfessel-Paxton		
✓ Use energy cuttoff	Initial energy cuttoff: 400 eV Increment: 22 eV		
The default for low preci	sion is 300.000 eV, the default for increased precision is 520.000 eV		
🗸 Use k spacing	Initial k spacing: 0.0575 Update factor: 0.9 Use	odd size grid	3
Corresponding k mesh 6	5 1 (0.051 0.052 0.035)		

Obtain Accurate Heats of Formation for SiC with ACFDT-RPA



Lattice parameters





Heats of formation





2nd. order 3rd. order

Introduction



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

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

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



1 Introduction

TUTORIA

WASP can derive the correlation energy expression in the random phase approximation (PFW) using the adiabatic connection fluctuation dissignation theorem (ACPDT) [J]. Harl and G. Kresse, Peys. Rev. B 77, 045156 (2008)], we extremely accurate method for the combination energy can be combined with the Hartmee-Fock exchange energy to derive a very accurate description of the exchange-correlation energy. Thereby providing a highly accurate ab INRo approach that predicts lattice constants and heats of formation with high accuracy and correctly considers wan 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.

1

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

Procedure Outline



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

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

ACFDT-RPA correlation ener Hartree-Fock total e Correction for partial occu	rgy: - energy: upancy:	12.219715 eV for Si2 -18.509282 eV for Si2 -0.000000 eV for Si2	ACFDT-RPA correlation energy Hartree-Fock total er Correction for partial occup	yy: Dergy: Dancy:	-27.34 -61 -0)385 eV fo. .141280 eV .000000 eV	r C4 for C4 for C4
ACFDT-RPA total e	energy:	-30.728997 eV for Si2	ACFDT-RPA total er	ergy:	-88	.490665 eV	for C4
Electronic contributions:	Empirical Formula Si	Cell (Si)8	Electronic contributions: En	npirical Form C	ula 	Cell (C)4	
ACFDT-RPA Energy	-1482.448	-11859.587 kJ/mol	ACFDT-RPA Energy	-2134.51	2 -8	3538.049 k	J/mol
ACFDT-RPA correlation ener Hartree-Fock total of Correction for partial occu	rgy: -: energy: upancy:	13.011143 eV for SiC -25.144840 eV for SiC -0.000000 eV for SiC			PBE	RPA	EXP
ACFDT-RPA total	energy:	-38.155983 eV for SiC		LiF	570	609	621
Electronic contributions:				NaF	522	567	576
1	Empirical Formula SiC	Cell (SiC)4		NaCl	355	405	413
ACFDT-RPA Energy	-3681.492			MgO	516	577	603
				MgH ₂	52	72	78
$\Delta H_f = E_{SiC} - E_{Si} - E_C$	=-3681.492-	+1482.448+2134.	512= -64.53 kJ/mol	AIN	262	291	321
				SiC	51	64	69

ACFDT-RPA: Computational Cost







ACFDT-RPA: Computational Cost





Scaling of low scaling RPA with k-points:





silicon

Conclusion



Tutorial showed how to use ACFDT-RPA to calculate the heat of formation

Calculated silicon carbide HoF is 64.5 kJ/mol

See also:

The Random Phase Approximation: A Practical Method Beyond DFT https://www.materialsdesign.com/webinars/recorded/ugm-2020-plenary-kresse

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



Interlude

MedeA VASP: Handling of Symmetry in Structures



Cu (Fm-3m)



Atom	Name	Element	Atomic Number	Wyckoff Position	Wyckoff Equatio
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



Cu (P1)



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 \rightarrow increase in calculation effort
- 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



▶ With symmetry: sites \neq atom positions



 Fe_3O_4 (Fd-3m)

Atom	Name	Element	Atomic Number	Wyckoff Position	Wyckoff Equation	x
1	0	0	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
	1	POSCAR:				
		(Fe3O4)8 1.0	(Fd-3m) ~	(Pearson	#1221350)_1	(VASP
			0.00000	000 4.1965	0000 4.1965	50000
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			4.19650	000 4.1965	0000 0.0000	00000
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		- (18910000	0 2297000	0 0 2297000) ()
		0	22970000	-0 1891000	0 0 2297000	0
		0	22970000	0.22970000	-0 1891000	
		0	.22970000	0.22970000	-0.1091000	
		0	. / / 030000	0.77030000	0.77030000)
		0	.18910000	0.//030000	0.77030000)
		0	. ///030000	0.18910000	0.77030000)
		0	.77030000	0.77030000	0.18910000)
		0	.00000000	0.00000000	0.0000000)
		\cap	50000000	0 0000000	0 0000000)

•••



MedeA VASP: Sites vs. Atom Positions





LDA+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





T [K]





Introduction



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

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

nduced	ectron Pho Change o a F	onon f the (functi	Cou GaAs on o	pling: s Ban of Terr	Phonoi d Gap a peratur Release 3.2
Objective: Learn 1 phonon-induced ter Modules: MindeA I	how to use the single disp imperature-dependent char WASP 6	facement app ige of the GaA	mach by Za a band gap	ichariaa and (WASP 6.	liustino to celculate I
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1 1 1 1		NOC.			
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Preparation time 30 minutes e: This tutorial can b ctures: GaAs F-43m.	Run time (4 Intel cores) 30 minutes e accelerated using the for sci	Level Intermediate	nd file:		
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Procedure Outline



1.Retrieve crystal structures of GaAs

- 2.Optimize the structure with PBEsol
- 3.Build a 1x1x1 supercell

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

- 4. Calculate the Zacharias-Giustino one-shot displacement pattern at 300 K
- 5. Obtain accurate band gaps with Modified Becke-Johnson LDA

Phonon Induced Temperature Dependent Change of the Anti-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 (Zacharia&Giustino)
 - Band gaps with MBJLDA



Introduction



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

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

Modules: MedeA VASP

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

	Cadmium	Seler	lide a	ind Ca	Sulfid Release 3.
· Objective: Learn	how to calculate the optic	al properties, s	such as the co	plor of materia	Ils using an <i>ab in</i>
Modules: MedeA	VASP				
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Preparation time 20 minutes Note: This tutorial CdS-P6.3mc CdSe-P6.3mc Dutline Calculate the Col Introduction	Pun time (4 Intel cores) Pon minutes can be accelerated using sci cso for of Cadmium Selenide au	Level Intermediate the following pr	epared structu	ure files.	
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Preparation time 20 minutes Note: This tutorial CdS-P6.3mc CdSe-P6.3mc Cutline Calculate the Col Introduction Proceed Retrieve the Define and	Pun time (4 Intel cores) Pon minutes can be accelerated using i sci csoi for of Cadmium Selenide au ure outline CdS (P8_mc) and CdSe (I Pun the Optical Properties	Level Intermediate the tollowing pr he tollowi	epared structu ultide	ure files:	
Preparation time 20 minutes Note: This tutorial CalS-P6.3mc CalSe-P6.3mc Calculate the Col Introduction Proceed Retrieve the Define and Analyze the	Pun time (4 Intel cores) To minutes can be accelerated using i sci sci cor of Cadmium Selenide au ure outline CdS (P8;mc) and CdSe (I Pun the Optical Properties Optical Spectra and View	Level Intermediate the following pr he followi	epared structu utilde from the Data	une files:	

MedeA VASP: Automated Calculation Protocol



						DFT	<pre>VASP 6 CALCULATION PROTOCOL: ====================================</pre>	step
culations	SCF: charge density			DT-RPA	Hartree-Fock	 Prepare for ACFDT-RPA by calculation of a large number of accurate excited states Calculate the ACFDT-RPA correlation energy 	,cep	
berty Calo	S	gap	pectra	nse ors	ACFI	Pre ACFDT-RPA	TFT	
Prop	Ö	Band	Optical S	Respo Tenso		ACFDT-RPA	Hartree-Fock	

Job.out:

Procedure Outline



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



CdSe CdS 🖒 Optical Spectra for 35485: (CdS)2 (P6_3mc) ~ 35482 minimized: (Pearson #1826218)_3 (VASP)- Color tutorial - MBJLDA A Optical Spectra for 35484: (CdSe)2 (P6_3mc) ~ 35483 minimized: (Pauling #454338)_4 (VASP)- Color tutorial - MBJLDA Optical spectra Color spaces Optical spectra Color spaces •••• T_x ••• T_x •• T_z ••• T_z — R_x — R x R_z 0.8-R_z •••• A_x ••• A_x •••• A_z A_z -0.4-0.4 0.4 Constanting the second Section 200 -0.2 -0.2 0.2 200 400 600 800 1000 300 600 900 1200 Wavelength (nm) Wavelength (nm) Material is a semiconductor Material is a semiconductor DC (Drude) Conductivity x: 0.0 eV Drude term: Not applied (for insulator or semiconductor) DC (Drude) Conductivity x: 0.0 eV Drude term: Not applied (for insulator or semiconductor) direct band gap = 1.87 eV direct band gap = 2.58 eV DC (Drude) Conductivity y: 0.0 Update and apply all settings eV Update and apply all settings Restore Drude conductivity DC (Drude) Conductivity y: 0.0 eV Restore Drude conductivity DC (Drude) Conductivity z: 0.0 Dielectric function (eps) Refractive index (n) Dielectric function (eps) Refractive index (n) eV DC (Drude) Conductivity z: 0.0 eV Inverse Drude Lifetime: 0.3 Conductivity (sig) Attenuation coefficient (a) Extinction coefficient (k) on coefficient (k) eV Inverse Drude Lifetime: 0.3 Co eV CdSe CdS Slab Thickness: 1000.0 Transmission coefficient (T) 🔽 Tri ivity (R) nm 000.0 nm Temperature: 2000.0 Blackbody radiation (BB) Spectral emi 2000.0 Bla vs. temperature 0.8 0.6 **MBJLDA** Exp. CdSe 0.4 CdS CdSe 1.87 eV 1.74 eV T(E) 0.2 A(E) CdS 2.58 eV 2.42 eV 0.0 800 300 400 500 600 700 31 band gap Wavelength [nm]

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 GGA 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



- 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

VASP 6	VASP 6 HT	Phonon	UNCLE	Mechanical Properties	Deformation	Effective Mass
		Calculation type: Full Brillouin zone Atom positions relaxed		Strains: 0.005	tension deformation Max strain: 0.2 (relative) in Z Strain increment: 0.01	Charge density from: previous stage k-Point: 0.0, 0.0, 0.0 Bands: +1 Grid: 3 Spacing: 0.0005 Ang^-1
+		+	+	÷	ł	Order. 2

List of Resources



Tutorials:

- Introduction to MedeA VASP: Learn how to set up and run VASP first principles calculations with MedeA
- Introduction to MedeA MT: Elastic Properties of TaN: Learn how to calculate the mechanical properties of crystals with MedeA MT and MedeA VASP
- Introduction to MedeA Phonon: Vibrational Properties of Silicon: Learn how to calculate the vibrational spectrum of silicon using MedeA Phonon with VASP and LAMMPS
- Introduction to MedeA UNCLE: Cluster expansion calculation of Au/Cu alloy: Learn how to set up cluster expansion calculations with MedeA UNCLE for Au/Cu alloy
- Introduction to MedeA FFO: Optimizing Buckingham Forcefield for LiNbO3: Learn how to optimize a Buckingham forcefield for LiNbO3 with MedeA Forcefield Optimizer
- Thermoelectrics: Seebeck Coefficient of Bismuth Chalcogenides: This tutorial describes how to calculate the Seebeck coefficient of the material Bi2Te3 with MedeA Electronics and MedeA VASP
- Calculate the Color of Cadmium Selenide and Cadmium Sulfide: Learn how to calculate the optical properties, such as color, of materials using an ab initio approach with MedeA VASP
- Electron-Phonon Coupling: Phonon Induced Change of the GaAs Band Gap as a Function of Temperature: 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 with MedeA VASP 6
- Obtain Accurate Heat of Formation for SiC with ACFDT RPA: Learn how to calculate the heat of formation of silicon carbide using ACFDT RPA with MedeA VASP 6
- Thermal Expansion of ZnO: Learn how to calculate the thermal expansion of materials with MedeA
- Webinars:
 - VASP in MedeA: A Fast Way- From Models to Reliable Results: <u>http://my.materialsdesign.com/webinar-31</u>
 - The Color of Materials: Value from Computed Optical Properties: <u>http://my.materialsdesign.com/webinar-25</u>
 - Atomistic Simulations as a Driver of Industrial Innovation: <u>http://my.materialsdesign.com/webinar-18</u>
 - Predicting Elastic Properties Using Ab Initio and Forcefield Based Simulations: <u>http://my.materialsdesign.com/webinar-15</u>

and more..

Materials Design UGM GOING GLOBAL October ugm.materialsdesign.com

Announcements

ugm.materialsdesign.com





Professor Rutger van Santen

Eindhoven University of Technology

Next Week's Plenary Speaker

October 22nd

Dr. René Windiks

Materials Design

MedeA Training

October 27th

More	Anr	nouncements			
JGM 2020 Forums		Q. Sec	irch 💮	Visit t	he UGM Forum page
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Training A Follow the training sessions, ask questions, post comments	© 0	口 0	Follow :	<	Ask questions

Technical Sessions

Additional resources, posters, and video presentations of scientific and technical research in the MedeA community.



poster

Risk Assessment of Drug Substance Tabletability using Quantum Mechanical Methods

In this work, periodic density functional theory as implemented in MedeA-VASP MT module was used to predict the mechanical properties of the single crystal structures of Vertex compounds along with other literature and small organic molecules in an automated manner



poster

The Color of Materials: Value from Computed Optical Properties

This poster provides guidelines for the calculation of the color of materials within the MedeA computational environment and illustrates the steps leading from the structure of



Contributor Volker Eyert

Announcements Visit the Technical Session page Submitted Talks and Posters

- There is still time to submit
- Open to customers under maintenance
- Easily upload on the contributor's page •
- Interested? Do you have questions? ٠
 - Contact Volker Eyert •
 - UGM@materialsdesign.com



Innovation by Simulation