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Question   Asked 11th Nov, 2017

Homnath Luitel
Variable Energy Cyclotron Centre

Can anybody suggest how to calculate the chemical potential of an element
using VASP?
I want to calculate the defect formation energy for different systems with defects
(both for atomic vacancies and doping impurity) using VASP.

I have found some papers from Physical Review Letters and Physical Review B
to calculate defect formation energy in different cases. But I am not getting how
to calculate the chemical potential of individual atoms using VASP.

| VASP | | Defects | | Doping | | Atomic | | Atoms |

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All Answers (5)

Andrey S. Mysovsky   11th Nov, 2017
Irkutsk State Technical University

It seems you are not the first person confused with that. I also spent some time
trying to understand where to get the correct chemical potentials.

The physically reasonable answer is: chemical potentials for each element
depend on the conditions of the experiment. If you carry, say, crystal annealing
in sodium vapour that increases the chemical potential for sodium. Quite
logically and even trivially, sodium from sodium vapour easily enters your
crystal, while in vacuum it does not.

So, the chemical potential for certain element depends on the chemical form in
which that element is present in the experimental conditions, on its
concentration and on the temperature.

This is why most people use total energies instead of honestly calculated
chemical potentials. Take the most widespread chemical form of your element
(say, O_2 for oxygen, metallic sodium for Na) and calculate total energy per one
atom. Use this value instead of chemical potential.

This is what I get thinking about this question and looking what other people do,
but, may be, someone can provide better answer.

2 Recommendations

Alexander Mironenko   11th Nov, 2017
University of Chicago

The "An Introduction to Applied Statistical Thermodynamics" book by Stanley
Sandler (or any other statistical mechanics book) contains expressions for
Gibbs free energies of an ideal gas (=chemical potential) that require
knowledge of temperature, pressure, vibrational frequencies, principal moments
of inertia, as well as the electronic energy of a given molecule, calculated
directly from VASP. I believe "Atomic Simulation Environment" platform (ASE)
has such expressions built-in and probably represents the most convenient way
to calculate chemical potentials using VASP. See https://wiki.fysik.dtu.dk/ase/.
Also, I suggest checking out the "ab initio thermodynamics" approach,
pioneered by M. Scheffler in early 2000's, for example, Reuter and Scheffler,
Physical Review B 65.3 (2001): 035406. They employ atomic chemical
potentials to calculate relative stability of material phases as a function of
reaction conditions.

2 Recommendations

Alexander Hofmann
Umicore

11th Nov, 2017

Hi there,

I like the explanations of Gaussian Inc. very much:

http://gaussian.com/thermo

They provide a detailed and step by step description of how to calculate each contribution to the chemical potential. They use the analytical expressions as well as give examples which help you understanding.

Alex

2 Recommendations

Homnath Luitel
Variable Energy Cyclotron Centre

11th Nov, 2017

Thank you all for your valuable suggestions!

1 Recommendation

Marsel Kaemo
studenten

6th Jun, 2018

hallo Hmnath,

I am new in this research. Can you tell me how you calculated chemical potential?

Can you help by adding an answer?

Answer

Add your answer

Add your answer

Does anyone know how to calculate chemical potential energy of hydrogen or halogens when GNR edges are functionalized with hydrogen or halogen atoms?

Question | 3 answers

Asked 10th Oct, 2015

Sadegh Mehdi Aghaei

--As you may know, the formation energy of a hydrogenated graphene nanoribbon can be calculated using

$E(f) = (E(ribbon) - n(C) \cdot E(C) - n(H) \cdot E(H2) / 2) / 2L$

E(pristine ribbon) : total energy of hydrogenated nanoribbons

E(H) and E(C): the total energy of free Hydrogen and CarbonL: the periodic length of the nanoribbon

--But this is for perfect vacuum conditions around freestanding graphene edges.

--In order to consider a molecular hydrogen gas atmosphere around the graphene edge (experimental conditions), the calculated total edge formation energy E(f) can be compared to the hydrogen chemical potential $\mu(H2)$, resulting in the relative edge stability (Gibbs free energy):

$G(H2) = E(f) - \rho(H) \cdot \mu(H2) /2$ ----> **Gibbs free energy**

where $\rho(H) = n(H) / 2L$ ----> **Edge hydrogen density**

$\mu(H2) = H0(T) - H0(0) - TS0(T) + kBT \ln (P/P0)$ ----> **Chemical Potential of H2 Molecule**

H: Enthalpy

S: Entropy

---Does anybody know how to calculate μ or chemical potential for **H or halogens** with above formula?

View

How could I make super cell and transform the coordinates of unit cell using VESTA?

Question   28 answers

Asked 10th Oct, 2015

👤 Garam Choi

Hello. Superiors.

I want to make super cell structure to calculate band structure.

I have been searching for it and found the paper attached (E.S.Tasci, "How to prepare an input file for surface calculation"). This paper was written to tell how to make super cell toward desired direction(means 'miller index') using VESTA program.

If you are familiar with VESTA or read this paper,

please help me for 2 problems below.

1. I made a primitive cell consisting of 2 atoms and changed it to 2x2x2 super cell in 'edit -> edit data -> unit cell' option. I expected I will get a super cell consisting of 16 atoms (2 atoms x 2x2x2 = 16 atoms) but I got 64 atoms or more after I exported the structure to POSCAR. Did I miss something important to get atoms and coordinates I want?

2. I am having hard time to understand how to transform the old coordinates to the new coordinates following by procedure explained in the paper attached. I can't match the result in the paper(the matrix in page 8) from originals (table 2). Could you explain it to me?

I have just started my study for DFT. So I hope I could get helps from this community.

Best regards,

View

What is the difference between LDOS and PDOS and how to visualize these using VASP?

Question   19 answers

Asked 3rd Mar, 2015

⚪ Shilendra Kumar Sharma

How to visualize the PDOS and LDOS after generating output files ?

View

How can I solve convergence Problems with VASP and large magnetic system?

Question   9 answers

Asked 11th Nov, 2016

⚪ Martin Baeker

I have a large (136 atoms) supercell consisting of two phases: An fcc

nickel part with 72 atoms and a Ni3-Ti-phase (eta phase).

The Nickel phase is ferromagnetic, whereas the eta phase is not.

When I run the system without magnetic

moments switched on

the calculation converges.

However, when I switch on magnetic moments, no convergence is reached.

Here is the relevant part of the INCAR file:

--- ENERGY ---

ENMAX=400

ENCUT=520

--- Simulation precision ---

PREC=Normal

LREAL=Auto

ROPT=1.e-4 1.e-4

ISMEAR=-5

#

--- Spin definition ---

ISPIN=2

MAGMOM= 128*5.0

#

--- KSPACING

KSPACING=0.2

KGAMMA=.TRUE.

NELM = 200

NELMDL=-10

NELMIN = 5

LMAXMIX=4

I have also tried to initialize only the Ni atoms with a magnetic

moment (MAGMOM=72*5. 64*0.), but this does not help convergence.

I also tried to first use the non-magnetic solution as a starting point, using

ISTART=1

ICHARG=1

ISPIN=2

MAGMOM= 128*5.0

in the continuation run, but this again does not help.

Furthermore, I tried different algorithms (using ALGO/IALGO), but did

not find any combination that worked for the system

Any ideas on how to get the system to converge (or how to nail down

the cause of the convergence issue) would be greatly appreciated.

View

How can I calculate formation energy using VASP-Ab-initio?

Question 4 answers

Asked 4th Apr, 2016

Rohit Pathak

How can I calculate formation energy of a system (unit cell of bulk/supercell thin film) by using ab-initio DFT method (VASP in particular)?

As per of my understanding suppose I want to calculate formation energy for bulk Fe_2VAl (gull Heusler alloy) then I should get it by using following $E_{form.} = E_{(Fe2VAl)} - 2*E_{Fe} - E_V - E_{Al}$

If its right then my question is that what value should I take it of E_{Fe}, E_V, and E_{Al}? Is it the energy value of Fe, V and Al calculated from a separate bulk calculation of Fe, V and Al for the respective crystal structure form in which they crystallizes individually or its some other value?

Please clarify my doubt, thanks in advance

sincerely

Rohit

View

What does formation energy mean?

Question 8 answers

Asked 5th May, 2014

Ezzah Azimah Alias

I had read some theoretical paper about defect in GaN. They analysis the defect using formation energies as a function of Fermi level. If the formation energy is too big, this defect is very unlikely to be seen. So what does this "formation energy" mean?

View

How to calculate formation energy using DFT?

Question 10 answers

Asked 12th Dec, 2013

Chandra Shekar

I want to calculate the formation energy of benzene, naphthalene, coronene. Is it measured in term of per atom (atom-1) ?

View

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First-principle study of extrinsic defects in CuScO2 and CuYO2

Article

May 2008

⬤ Zhi-Jie Fang · ⬤ Li-Jie Shi

Using first-principles methods, we studied the extrinsic defects doping in transparent conducting oxides CuMO2 (MSc, Y). We chose Be, Mg, Ca, Si, Ge, Sn as extrinsic defects to substitute for M and Cu atoms. By systematically calculating the impurity formation energy and transition energy level, we find that BeCuBeCu is the most prominent extrinsic...

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Defect-Based Single-Atom Electrocatalysts

Article

Dec 2018

⬤ Yiqiong Zhang · ⬤ Lan Guo · ⬤ Li Tao · [...] · ⬤ Shuangyin Wang

Single-atom catalysts (SACs) have attracted great attention owing to their maximum atomic utilization and high catalytic performance in electrochemical reactions. But the synthesis of SACs is not easy due to large surface energies of single atomic metal sites which often lead to their aggregation. The defects on supports can serve as anchor sites t...

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Comparing two iteration algorithms of Broyden electron density mixing through an atomic electronic structure computation

Article

May 2016

⬤ Man-Hong Zhang

By performing the electronic structure computation of a Si atom, we compare two iteration algorithms of Broyden electron density mixing in the literature. One was proposed by Johnson and implemented in the well-known VASP code. The other was given by Eyert. We solve the Kohn-Sham equation by using a conventional outward/inward integration of the di...

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