

Manual for sxdefectalign version 3.0

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You want to ...

... **quickly proceed to using sxdefectalign?**

Start by the examples in Sec. 4.

... **understand the command-line options?**

See Sec. 2.

... **process output files?**

See Sec. 3.

... **see equations?**

Read from Sec. 1.2 onward.

... **get support for a new DFT code?**

Check out Sec. 5.

... **see what's new?**

See list of changes in Sec. 1.1.

The general formalism is described in Ref. [1]. The present version contains a bug fix concerning the alignment constant Δ_q [2]: instead of calculating it from the short-range average, it is set to $-C$ to take into account alignments that do not arise from charging effects, e.g. from pseudopotentials.

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1 Description

1.1 Changes

1.1.1 Changes since version 2.2

- support for mixed screening corrections (vertical transitions from pre-charged states, configuration coordinate diagrams), see Sec. 2.2.
- support for multiple charges
- experimental ionic core fitting
- support socorro and quantum espresso/cube files in Hartree

1.1.2 Changes since version 2.1

- the `vAtoms.dat` column order has changed
- support for quantum espresso file format

1.1.3 Changes since version 1.3

- support for dielectric tensors
- atomic sphere averages
- support for socorro file format
- planar averages are computed along all 3 cell vectors, into `vline-eV-a0.dat`, `vline-eV-a1.dat`, and `vline-eV-a2.dat`.

1.2 Implementation details

The charge model presently supported by `sxdefectalign` is

$$q_d(r) = qxN_\gamma e^{-r/\gamma} + q(1-x)N_\beta e^{-r^2/\beta^2}, \quad (1)$$

where N_γ and N_β are appropriate normalization constants, and q is the charge¹. In reciprocal space, it reads (excluding the Fourier normalization constant)

$$q_d(g) = \frac{qx}{(1+\gamma^2g^2)^2} + q(1-x)e^{-\frac{1}{4}\beta^2g^2} \quad (2)$$

The unscreened electrostatic self-energy for a single charge is computed as

$$E^{\text{iso}} = \frac{1}{2} \frac{1}{(2\pi)^3} \int d^3\mathbf{g} \frac{4\pi}{|\mathbf{g}|^2} [q_d(|\mathbf{g}|)]^2 = \frac{1}{\pi} \int_0^{g^{\text{cut}}} dg [q_d(g)]^2. \quad (3)$$

¹**Note:** most DFT codes define potentials for the electrons, not for classical test charges. For consistency, the charge q must be given in units of electrons (i.e. a +1 defect has -1 electrons).

If the model charge consists of multiple charges, there are additional pair-wise interaction energies, which can be computed as

$$\begin{aligned} E^{\text{iso}:i/j} &= \frac{1}{(2\pi)^3} \int d^3 \mathbf{g} \frac{4\pi}{|\mathbf{g}|^2} j_0(|\mathbf{g}| r_{ij}) q_d^i(|\mathbf{g}|) q_d^j(|\mathbf{g}|) \\ &= \frac{2}{\pi} \int_0^{g_{\text{cut}}} dg j_0(g r_{ij}) q_d^i(g) q_d^j(g), \end{aligned} \quad (4)$$

where j_0 denotes the spherical Bessel-function for $l = 0$ (i.e. $j_0(x) = \sin(x)/x$), and r_{ij} is the distance between the charges i and j . $q_d^{(i)}$ denotes the charge shape for the i -th charge (each charge may have its own Gaussian width and exponential tail).

The periodic energy is computed as (Ω denotes the unit cell volume)

$$\frac{2\pi}{\Omega} \sum_{\mathbf{G} \neq 0, |\mathbf{G}| \leq g_{\text{cut}}} \frac{[q_d(|\mathbf{G}|)]^2}{|\mathbf{G}|^2} + \frac{q}{\sqrt{\Omega}} V(0), \quad (5)$$

where the second term is the alignment correction for the model charge array. For multiple charges, q_d in Eq. (5) is replaced by the total charge density

$$q_d^{\text{tot}}(\mathbf{g}) = \sum_i q_d^{(i)}(\mathbf{g}) e^{-i\mathbf{g} \cdot \boldsymbol{\tau}^i} \quad (6)$$

where $\boldsymbol{\tau}^i$ denotes the position of the i -th charge.

In contrast to the original paper, the alignment correction of the model charge density is included in the periodic energy, because lattice energies of non-overlapping models then agree with the point-charge result (provided that the potentials are aligned) [2]. The average electrostatic potential along the sample direction a reads

$$V(G_a \neq 0) = \frac{4\pi}{\sqrt{\Omega}} \frac{q_d(G_a)}{|G_a|^2} e^{-iG_a \tau_a} \quad (7)$$

with τ being the position of the defect center, while

$$V(0) := \frac{2\pi}{\sqrt{\Omega}} \left. \frac{d^2 q_d(g)}{dg^2} \right|_{g=0}. \quad (8)$$

This convention ensures a constant alignment of the potential as the model parameters x , β , and γ , are varied. The real-space average potential is obtained from a Fourier series

$$\bar{V}(r_a) = \frac{1}{\sqrt{\Omega}} \sum_{G_a} V(G_a) e^{iG_a r_a}. \quad (9)$$

For multiple charges, the potential contributions of each charge are summed.

The short-range potential V^{sr} is obtained from the above long-range model potential and the actual local electrostatic potentials from the defect and reference DFT calculations as

$$V^{\text{sr}} = V^{\text{DFT}}(\text{defect}) - V^{\text{DFT}}(\text{reference}) - V(\text{long-range model}) . \quad (10)$$

Please note that we require that the supercell of the defect is an exact multiple of the reference supercell, i.e., **no lattice relaxation is allowed**.

The full source code is part of the S/PHI/nX package², which is freely available at <https://sxrepo.mpie.de>.

1.3 Anisotropic screening

Originally, the scheme was developed for isotropic screening. In this case, the unscreened energies and potentials are simply scaled by the inverse dielectric constant.

Anisotropic screening requires to use a dielectric tensor $\underline{\epsilon} = \epsilon_{\alpha\beta}$, where α and β are cartesian indices (x, y, z) [3]. Dielectric tensors are specified using the `--tensor` option instead of the `--eps` option. If your dielectric tensor is aligned to the coordinate system (all off-diagonal elements = 0), it is sufficient to provide the diagonal elements. If you provide 6 elements, these define the dielectric tensor in Voigt notation: $\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, \epsilon_{yz}, \epsilon_{xz}, \epsilon_{xy}$. If you provide 9 elements, you give the dielectric tensor (which must be symmetric!) in its 3×3 representation row by row: $\epsilon_{xx}, \epsilon_{xy}, \epsilon_{xz}, \epsilon_{xy}, \epsilon_{yy}, \epsilon_{yz}, \epsilon_{xz}, \epsilon_{yz}, \epsilon_{zz}$.

However, we follow a different approach than Kumagai and Oba [3] for evaluating the anisotropically screened energy. The screened periodic potential reads³

$$V(\mathbf{G} \neq \mathbf{0}) = \frac{4\pi}{\sqrt{\Omega}} \frac{q_d(\mathbf{G})}{\mathbf{G}^\dagger \underline{\epsilon} \mathbf{G}} \quad (11)$$

and we use the alignment convention for $\mathbf{G} = \mathbf{0}$

$$V(0) := \frac{2\pi}{\bar{\epsilon}\sqrt{\Omega}} \left. \frac{d^2 q_d(g)}{dg^2} \right|_{g=0} . \quad (12)$$

Here, $\bar{\epsilon}$ is the appropriate spherical average from

$$\frac{1}{\bar{\epsilon}} = \frac{1}{4\pi} \int d\hat{\mathbf{g}} \frac{1}{\hat{\mathbf{g}}^\dagger \underline{\epsilon} \hat{\mathbf{g}}} \quad (13)$$

where the integration in $\hat{\mathbf{g}}$ is over the unit sphere. In practice, we determine it from a 110-point Lebedev spherical grid [4]. The screened periodic energy reads

$$E = \frac{1}{2\sqrt{\Omega}} \sum_{\mathbf{G} \neq \mathbf{0}} V(\mathbf{G}) q_d(|\mathbf{G}|) + \frac{q}{\sqrt{\Omega}} V(0) , \quad (14)$$

²The source is in `sphinx/src/tools/SxDefectAlign.cpp`, but makes heavy use of the S/PHI/nX libraries, so you cannot compile it without S/PHI/nX.

³In the denominator, $\mathbf{G}^\dagger \underline{\epsilon} \mathbf{G} = \sum_{\alpha\beta} G_\alpha \epsilon_{\alpha\beta} G_\beta$

The isolated energy is obtained from the spherically averaged screening, i.e., from Eq. (3) scaled by $1/\bar{\epsilon}$.

For multiple charges, there is an additional pairwise anisotropy term in the isolated energy, that can be derived by expanding the plane-waves in spherical harmonics. This term reads for each charge pair

$$E^{\text{aniso}:i/j} = \frac{2}{\pi} \sum_{l=2}^{l_{\text{max}}} i^l \left[\int_0^{g_{\text{cut}}} dg j_l(g|r_{ij}) q_d^{(i)}(g) q^{(j)}(g) \right] \times \sum_{m=-l}^l Y_{lm} \left(\frac{\tau^j - \tau^i}{r_{ij}} \right) \int d\hat{\mathbf{g}} \frac{Y_{lm}^*(\hat{\mathbf{g}})}{\hat{\mathbf{g}}^\dagger \underline{\epsilon} \hat{\mathbf{g}}}. \quad (15)$$

Only even l contribute due to symmetry. The $l = 0$ term corresponds to the isotropic pair-wise contribution Eq. (4) screened by the isotropically averaged dielectric constant $\bar{\epsilon}$. In practice, we use $l_{\text{max}}=12$, and a 230-point Lebedev grid [5] for spherical integration. The pairwise interactions in the periodic energy are naturally included by using potential and charge in Eq. (14) that contain all charge contributions.

Please note that the dielectric anisotropy is less extensively tested; I would greatly appreciate feedback if you use it. Preliminary tests on weakly anisotropic systems ($\sim 10\%$ difference in the main components of the dielectric tensor) showed a marginal change in the calculated correction, while slightly improving the agreement for the alignment in the different directions. For these cases, the effort of determining the dielectric tensor may not be worthwhile. For more strongly anisotropic systems (e.g. layered systems), treating the dielectric anisotropy is a must [3].

1.4 Vertical transitions, configuration coordinate diagrams with mixed screening

If the ionic contribution to the total screening is important, special corrections apply when the geometry has been obtained for a charge state, but the final calculations has been made for a different charge state, e.g. when computing vertical transitions. In this case, a mixed screening charge correction is needed [8, 9] by considering two subsequent charging steps: first, the "initial" charge $q_1(\mathbf{r})$ with full ionic and electronic screening ϵ_0 in the potential V_1 and second, the extra charge q_2 with electronic screening ϵ_∞ in the potential V_2 only. For the final state, the electrostatic correction becomes

$$E^{\text{corr}} = E^{\text{iso}} - E^{\text{periodic}} + (q_1 + q_2)C \quad (16)$$

with

$$E^{\text{periodic}} = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G} \neq \mathbf{0}} \left[\frac{1}{2} q_1(\mathbf{G})^* V_1(\mathbf{G}) + q_2(\mathbf{G})^* V_1(\mathbf{G}) + \frac{1}{2} q_2(\mathbf{G})^* V_2(\mathbf{G}) \right] + \frac{2\pi}{\sqrt{\Omega}} \left(\frac{1}{\epsilon_0} q_1(0) \left. \frac{d^2 q_1(g)}{dg^2} \right|_{g=0} + \frac{1}{\epsilon_0} q_1(0) \left. \frac{d^2 q_2(g)}{dg^2} \right|_{g=0} \right)$$

$$\left. + \frac{1}{\epsilon_0} q_2(0) \frac{d^2 q_1(g)}{dg^2} \right|_{g=0} + \frac{1}{\epsilon_\infty} q_2(0) \frac{d^2 q_2(g)}{dg^2} \right|_{g=0} \Bigg). \quad (17)$$

For the reciprocal-space charges $q(\mathbf{g})$ and potentials $V(\mathbf{G})$, see Sec. 1.2 and Sec. 1.3. The total model potential is $V^{\text{lr}} = V_1 + V_2$, the $\mathbf{G} = \mathbf{0}$ component is

$$V(0) = \frac{2\pi}{\epsilon_0 \sqrt{\Omega}} \left. \frac{d^2 q_1(g)}{dg^2} \right|_{g=0} + \frac{2\pi}{\epsilon_\infty \sqrt{\Omega}} \left. \frac{d^2 q_2(g)}{dg^2} \right|_{g=0}.$$

This potential is used for determining the alignment constant in the same way as for the standard corrections.

For the isolated energy, we use Eq. (3) for the individual charges' self energy $E^{\text{iso}}[q_n^i]$ ($n=1$ or 2), with prefactor $\frac{1}{\epsilon_0}$ for all single charges contained in q_1 , and a prefactor of $\frac{1}{\epsilon_\infty}$ for those in q_2 . If q_1 and q_2 contain more than a single charge, the interactions between the single charges inside q_1 and q_2 , respectively, are computed via Eq. (4). It is absolutely fine to work with single charges. Eq. (4) is also used for the interaction between all individual charges belonging to q_1 and q_2 , respectively. Thus, for N_1 many charges in q_1 and N_2 many charges in q_2 ,

$$\begin{aligned} E^{\text{iso}} &= \frac{1}{\epsilon_0} \sum_i^{N_1} E^{\text{iso}}[q_1^i] + \frac{1}{\epsilon_\infty} \sum_i^{N_2} E^{\text{iso}}[q_2^i] \\ &+ \frac{1}{\epsilon_0} \sum_i^{N_1} \sum_j^i E^{\text{iso}}[q_1^i, q_1^j] + \frac{1}{\epsilon_\infty} \sum_i^{N_2} \sum_j^i E^{\text{iso}}[q_2^i, q_2^j] \\ &+ \frac{1}{\epsilon_0} \sum_i^{N_1} \sum_j^{N_2} E^{\text{iso}}[q_1^i, q_2^j] \end{aligned} \quad (18)$$

In order to distinguish the charges belonging to q_1 and q_2 , we use the `--vertical-eps` option, that sets ϵ_∞ , as a separator. All charges appearing before `--vertical-eps` belong to q_1 , all charges after `--vertical-eps` belong to q_2 . Due to my laziness in coding special cases in command line parsing, you must repeat the charge position with the `--pos` option for q_2 , even if it doesn't change from q_1 .

1.5 Atomic sphere averages

The original scheme for evaluating the shift in the potential from planar averages works nicely for systems dominated by electronic screening, but gets painful when ionic screening becomes important. The main reason is that as ions move between the defect and reference system, the strong contribution from the ionic core does not cancel, leading to wild oscillations in the potential difference. While this can be damped partly by averaging, the present version offers an alternative scheme: evaluation of the potential near the ionic cores (similar to [3]). In practice, we compute the potential average around each atom with a

Gaussian weight function. As the center of the Gaussian moves with the atom, the ionic cores largely cancel out.

The spherical average for an atom located at τ' is obtained from

$$\bar{V}_{\tau'} = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G} \neq 0, |\mathbf{G}| \leq g_{\text{cut}}} V(\mathbf{G}) e^{i\mathbf{G}\tau'} e^{-\frac{1}{2}|\mathbf{G}|^2\beta^2} \quad (19)$$

where the Gaussian broadening β defaults to 1.5 bohr; it can be changed via the `--atomAverage` option.

Atomic sphere averages are automatically computed if the atomic positions are available (VASP, socorro, quantum espresso, SPHInX structure files). In practice, we map defect atoms to the bulk atoms with a tolerance of 0.5 bohrs in the coordinates.

1.6 Removing ionic core potentials

Since version 3.0, `sxdefectalign` includes an algorithm for smoothening the electrostatic potential by subtracting ionic cores similar to the approach of Sundaraman and Ping [7], except that we fit the ionic core shapes on the fly. Details are described elsewhere [10]. This is slow, so use only when needed. In my experience, core fitting efficiently dampens oscillations in the plane-averaged potential profiles at the length scale of the ionic core (1-3 bohrs), but adds high-frequency noise due to the comparatively sharp cutoff. Therefore, combination with window-averaging (`--average`) is highly recommended.

2 Options

Option	argument	description
--help		show all the available options
--ecut	energy	reciprocal space cutoff energy (Ry). This implicitly defines the Fourier mesh size.
--eps	ϵ	dielectric constant
--tensor	$\epsilon_{\alpha\beta}$	dielectric tensor.
--pos	x,y,z	center of defect (default: bohr)
--relative		center of defect is in relative coordinates
--charge	q	defect charge in charge units used by the DFT program (note: most programs use q(electron) = +1, so q must be minus classical charge)
--beta	β	changes the width of the Gaussian $e^{-\beta^2/r^2}$ (bohr)
--gamma	γ	exponential decay constant
--expnorm	x	relative amount of exponential decay (0..1)
--vref	file	reference potential (bulk)
--vdef	file	defect potential
--vasp		all potentials are VASP LOCPOT files
--socorro		all potentials are socorro files
--qe		all potentials are quantum espresso files. The potential reader is being tested right now. Report any trouble with it!
--average	width	average in order to smoothen wiggly potentials (bohr)
--format [=format]		specify output format for line profiles: xmgrace, separate, or matrix, see Sec. 3
-C	alignment	shift long-range potential (eV)
--structDef	file	structure file (SPHInX format) for defect
--structRef	file	structure file (SPHInX format) for reference
--atomAverage	width	Gaussian broadening for atomic-sphere averages (bohr)
--anticore[=options]		apply ionic core fitting. You may specify up to three comma-separated parameters in the following order: the ionic core cutoff radius (in bohr), the number of sampling points, and the spline order.

2.1 Multiple charges

To specify a complex model charge that consists of several individual charges, you may use the `--pos` option multiple times. To adapt the charge, β , γ , and x parameters for an individual charge, specify these *after* the position. If these values are not set, the charge and Gaussian width are kept from any previous setting, while the exponential tail is reset to zero.

2.2 Mixed screening

Option	argument	description
<code>--eps</code>	ϵ_0	full dielectric constant
<code>--vertical-eps</code>	ϵ_∞	electronic dielectric constant or tensor. If tensor, it uses the same format as for <code>--tensor</code>

Charges appearing before the `--vertical-eps` are subject to full screening, charges appearing thereafter only to electronic screening. Note that we provide final-state corrections, to obtain corrections for the transition only, subtract the correction of the fully screened initial state.

Mixed screening is compatible with anisotropic screening, just use `--tensor` instead of `--eps`.

Since mixed screening uses multiple charges, the position of the defect charge *must always* be given by starting with the `--pos` option, before giving any further details such as the charge or the exponential tail. The position *must* be repeated directly after `--vertical-eps` option.

3 Output

3.1 Planar averages: `vline-eV-a{0,1,2}.dat`

3.1.1 Traditional 'xmgrace' format:

`vline-eV-a{0,1,2}.dat`, an xmgrace-style file, containing

```
z V(long-range)
...
&
z V(defect)-V(ref) V(defect)-V(ref)-V(long-range)
...
```

where z (in bohr) is the coordinate along the profiling axis, and $V(\cdot)$ is the planar average over the other two axes. In other words, there is a two-column set and a three column set. The third column of the second set is the short-range potential.

3.1.2 New formats

To simplify parsing with other programs, we offer two alternative formats accessible via the `--format` option: `'separate'` and `'matrix'`.

`'separate' format` contains the data set as a series of two-columns separated by newlines:

```
z V(long-range)
...

z V(defect)-V(ref)
...
```

```
z V(defect)-V(ref)-V(long-range)
```

```
...
```

'matrix' format contains the entire data set as a single 4 column block:

```
z V(long-range) V(defect)-V(ref) V(defect)-V(ref)-V(long-range)
```

```
...
```

3.2 Atomic sphere averages: vAtoms.dat

When structures and potentials are provided, there is a file `vAtoms.dat`. The format is⁴

```
r V(long-range) V(defect)-V(ref) V(defect)-V(ref)-V(long-range) x y z
```

```
...
```

with one line per atom in the defect cell that could be successfully mapped to the reference structure (tolerance: 0.5 bohr). Here, `r` is the distance from the defect center (in bohr), `V(...)` are spherical-Gaussian averaged potentials, and `x,y,z` are the coordinates of the atom in the defect cell. They are sorted by species, with an empty line separating the different chemical species.

For multiple charges, the defect center is set from the first charge. If this is not appropriate, I suggest to introduce a zero charge as the first one to set the defect center without affecting the energy or potential.

4 Usage

Note: After downloading the executable, make sure that the executable bit is set via

```
chmod u+x sxdefectalign
```

and that the current directory (`.`) is in your `PATH`. Otherwise, mark the path with `./sxdefectalign`.

The procedure is to run the program once without `-C` parameter, check that the short-range potential reaches a plateau, and read off the plateau value `C`. Then run the program a second time, with `-C C` and take the correction from the output. The correction printed out must be added to the uncorrected formation energy.

4.1 Example: SPHInX

Assume you have two directories: one `vacancy/` that contains the calculation of a vacancy, and `bulk/` that contains an equivalent bulk calculation. Both

⁴The order of columns has changed from version 2.1 to 2.2: the long-range and `V(defect) - V(ref)` columns have been swapped.

calculations were run with a 40 Ry cutoff. The vacancy is in the +2 charge state (i.e. -2 electrons). The vacancy sits in the center of the cell. The dielectric constant of the host material is 8.9. Then use the following single line

```
sxdefectalign --ecut 40 --charge -2 --eps 8.9 --center 0.5,0.5,0.5 --relative
--vdef vacancy/vElStat-eV.sxb --vref bulk/vElStat-eV.sxb
```

to create `vline-eV-a0.dat`, `vline-eV-a1.dat`, and `vline-eV-a2.dat`. I use `xmgrace` for plotting the data (you may use any other program, of course).

```
xmgrace -nxy vline-eV-a0.dat
```

Looking at the plot, you read off a plateau value of $C=-0.12$ eV for the green line. Thus you run

```
sxdefectalign --ecut 40 --charge -2 --eps 8.9 --center 0.5,0.5,0.5 --relative
--vdef vacancy/vElStat-eV.sxb --vref bulk/vElStat-eV.sxb -C -0.12
```

to get the final output. The correction is added to the formation energy.

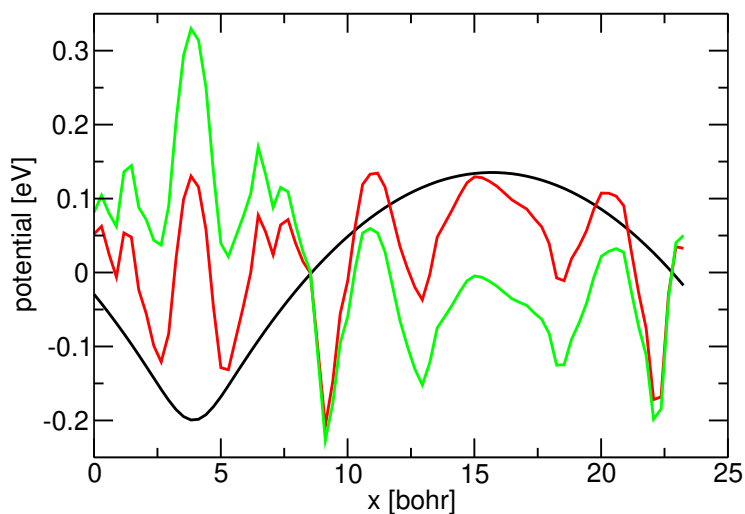
4.2 Example: SPHInX - vacancy in MgO

Assume you have two directories: one `vacancy/` that contains the calculation of a vacancy, and `bulk/` that contains an equivalent bulk calculation. Both calculations were run with a 40 Ry cutoff. The vacancy is in the +2 charge state (i.e. -2 electrons). The vacancy sits in relative position $[\frac{1}{6}, \frac{1}{6}, \frac{1}{6}]$ of the cell. The dielectric constant of the host material is 9.8. Then use the following single line

```
sxdefectalign --ecut 40 --charge -2 --eps 9.8 --center 0.1667,0.1667,0.1667 --relative
--vdef vacancy/vElStat-eV.sxb --vref bulk/vElStat-eV.sxb
```

to create `vline-eV-a0.dat`, `vline-eV-a1.dat`, and `vline-eV-a2.dat`. I use `xmgrace` for plotting the data (you may use any other program, of course).

```
xmgrace -nxy vline-eV-a0.dat
```

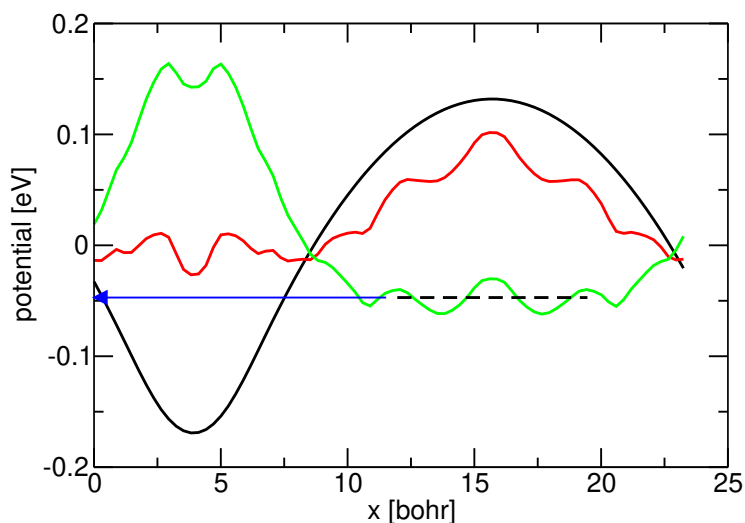


Alignment plot with no averaging.

Looking at the plot, we notice that we "drown" in oscillations. The reason is that MgO has a strong ionic screening, and when the deep ionic potentials move, their contributions in the defect and the bulk reference do not cancel. One approach is to dampen the oscillations by averaging. In this particular case, the oscillations "period" seems to be coupled to the atomic layers (separated at 3.92 bohr), so we use the following extra option in a new run:

`--average 3.92`

and obtain the following plot



Alignment plot with window averaging (3.92 bohr).

Looking at the plot, we estimate a plateau value (dashed line) of $C=-0.05$ eV.
Thus you run

```

sxdefectalign --ecut 40 --charge -2 --eps 9.8 --center 0.1667,0.1667,0.1667 --relative
--vdef vacancy/vElStat-eV.sxb --vref bulk/vElStat-eV.sxb -C -0.05

```

to get the final output:

```

+-----+
=== Intermediate results (unscreened) ===
Isolated energy      : 1.59577
Periodic energy      : 1.35472
Difference (Hartree)  : -0.241048
Difference (eV)      : -6.55926
+-----+
Calculation performed with epsilon = 9.8
+-----+
Defect correction (eV): 0.569313 (incl. screening & alignment)

```

The correction in the last line (i.e. 0.57 eV) is then added to the formation energy.

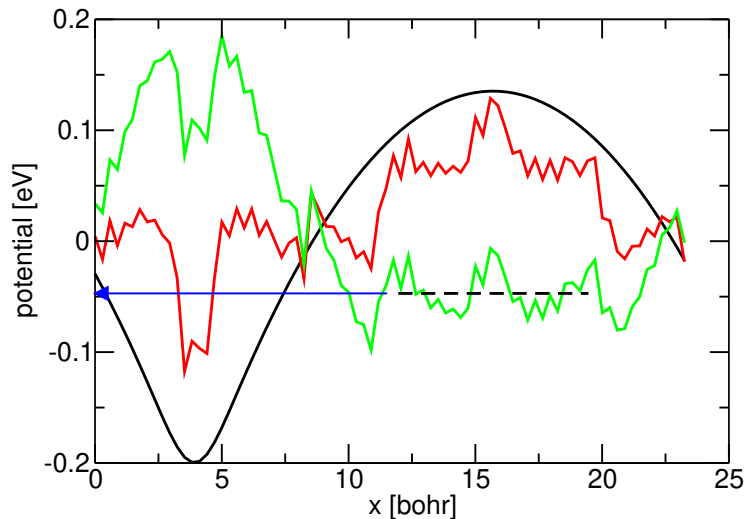
As an alternative to window averaging, we can also use the core removal

```

--anticore --structDef vacancy/relaxedStr.sx --structRef bulk/input.sx

```

The `--structDef` and `--structRef` options provide the atomic structure for SPHInX, since SPHInX doesn't encode them automatically in the potential files – in contrast to VASP, socorro, and quantum espresso. The plot becomes

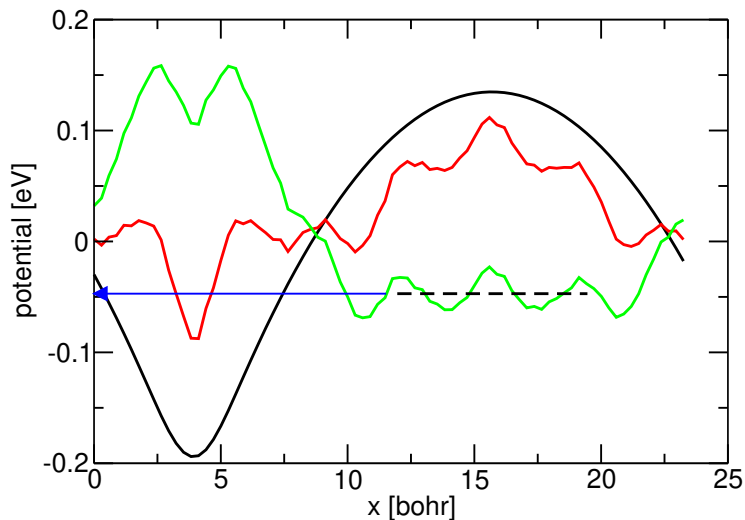


Alignment plot with ionic core removed (no averaging).

Looking at the plot, one clearly sees the high-frequency noise from the ionic core cutoff. To remove it, we can use a sufficiently large window averaging, e.g.

```
--anticore --structDef vacancy/relaxedStr.sx --structRef bulk/input.sx --average 1.5
```

with this result:

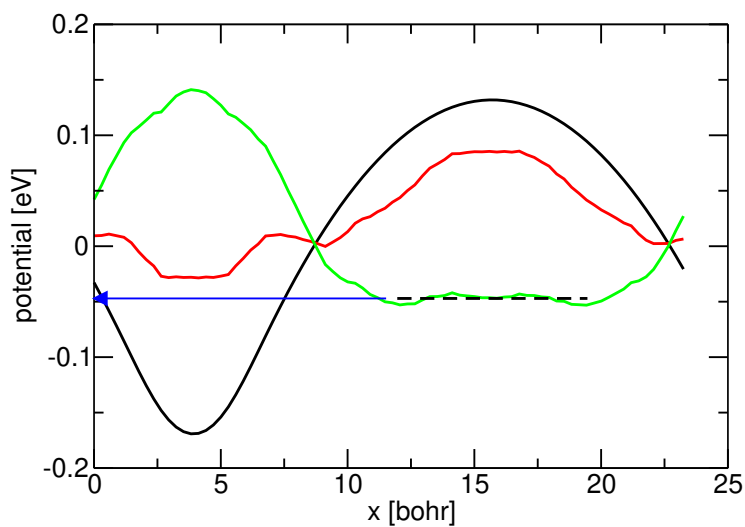


Alignment plot with ionic core removed (1.5 bohr averaging).

The optimal result is obtained when combining with an averaging matched to the interlayer distance of 3.92 bohr:

```
--anticore --structDef vacancy/relaxedStr.sx --structRef bulk/input.sx --average 3.92
```

with this result:



Alignment plot with ionic core removed and 3.92 bohr averaging.

Note that in alignment plots shown above, the alignment value and hence the correction is the same. The main difference is the uncertainty with which it is determined. Hence, it is not necessary to play with the parameters until you get a perfect result, as long as you are confident in the accuracy of the alignment value⁵.

4.3 Example: VASP

Assume you have two directories: one `vacancy/` that contains the calculation of a vacancy, and `bulk/` that contains an equivalent bulk calculation. Both calculations were run with a 400 eV cutoff (≈ 30 Ry). The vacancy is in the +2 charge state (i.e. -2 electrons). The vacancy sits in the center of the cell. The dielectric constant of the host material is 8.9. Then use the following single line

```
sxdefectalign --ecut 30 --charge -2 --eps 8.9 --center 0.5,0.5,0.5 --relative
--vdef vacancy/LOCPOT --vref bulk/LOCPOT --vasp
```

to create `vline-eV-a0.dat`, `vline-eV-a1.dat`, and `vline-eV-a2.dat`. I use `xmgrace` for plotting the data (you may use any other program, of course).

```
xmgrace -nxy vline-eV-a0.dat
```

Looking at the plot, you read off a plateau value of $C = -0.12$ eV for the green line. Thus you run

```
sxdefectalign --ecut 30 --charge -2 --eps 8.9 --center 0.5,0.5,0.5 --relative
--vdef vacancy/LOCPOT --vref bulk/LOCPOT --vasp -C -0.12
```

to get the final output. The correction is added to the formation energy.

4.4 Example: socorro

This example is a Ga vacancy in GaAs in the -3 charge state (i.e. +3 electrons), including ionic relaxation. Assume you have two files for the electrostatic potential: `els_potential_defect` and `els_potential_bulk`. We will use a plane-wave cutoff of 20 Ry. The vacancy sits in the origin of the cell. The dielectric constant of the host material is 12.9. As the ions move, the raw potential difference is very wiggly. We will therefore use a 5.2 bohr averaging. Then use the following single line

```
sxdefectalign -q 3 --eps 12.9 --vdef els_potential_defect
--vref els_potential_bulk --ecut 20 --socorro --average 5.2
```

to create `vline-eV-a0.dat`, `vline-eV-a1.dat`, and `vline-eV-a2.dat`. I use `xmgrace` for plotting the data (you may use any other program, of course).

⁵The recurrent need to fine-tune the averaging procedure in a case-to-case manner and judge the quality by human inspection is the main reason why I currently do not provide any "automatic" alignment.


```
xmgrace -nxy vline-eV-a0.dat
xmgrace -nxy vline-eV-a1.dat
xmgrace -nxy vline-eV-a2.dat
```

Looking at the plots, you estimate a plateau value of $C=-0.01$ eV for the green line. Thus you run

```
sxdefectalign -q 3 --eps 12.9 --vdef els_potential_defect
--vref els_potential_bulk --ecut 20 --socorro --average 5.2 -C -0.01
```

to get the final output. The correction is added to the formation energy.

4.5 Example: quantum espresso

This example is a Ga vacancy in GaAs is in the -3 charge state (i.e. +3 electrons), including ionic relaxation. We will use a plane-wave cutoff of 30 Ry. In quantum espresso, one first uses the `pw.x` executable to do the DFT calculation for the pristine and defected structures and then use the `pp.x` executable to get the potential as a cube file[6].

Example input for the generation of the cube file:

```
&INPUTPP
  prefix='GaAs'
  outdir='relax_pris'
  filplot='relax_pris.pp'
  plot_num = 11
/
&PLOT
  nfile=1
  filepp(1)='relax_pris.pp'
  iflag=3
  output_format=6
  fileout='v_elec_pristine.cube'
/
```

Assume you have two files for the electrostatic potential: `v_elec_defect.cube` and `v_elec_pristine.cube`.

The vacancy sits in the origin of the cell. The dielectric constant of the host material is 12.9. As the ions move, the raw potential difference is very wiggly. We will therefore use a 5.2 bohr averaging. Then use the following single line

```
sxdefectalign -q 3 --eps 12.9 --vdef v_elec_defect.cube
--vref v_elec_pristine.cube --ecut 30 --qe --average 5.2
```

to create `vline-eV-a0.dat`, `vline-eV-a1.dat`, and `vline-eV-a2.dat`. I use `xmgrace` for plotting the data (you may use any other program, of course).

```
xmgrace -nxy vline-eV-a0.dat
xmgrace -nxy vline-eV-a1.dat
xmgrace -nxy vline-eV-a2.dat
```

Looking at the plots, you estimate a plateau value of $C=-0.01$ eV for the green line. Thus you run

```
sxdefectalign -q 3 --eps 12.9 --vdef v_elec_defect.cube
--vref v_elec_pristine.cube --ecut 30 --qe --average 5.2 -C -0.01
```

to get the final output. The correction is added to the formation energy.

5 Potential file formats

At present, `sxdefectalign` supports SPHInX, VASP, socorro, and quantum espressopotential files. For other programs, you have to generate the defect and reference profiles yourself. To set the supercell dimensions from the command line, use the following command line options.

```
--axis1 "x1,y1,z1" --axis2 "x2,y2,z2" --axis3 "x3,y3,z3"
```

Please note that the alignment correction of the model potential is included in the periodic energy. The defect alignment constant can then be provided with the `-C` option to obtain the total correction.

Alternatively, you can help me to implement support for your files into the program. For this, send a package to freysoldt@mpie.de with

1. Name of the code (or potential file type)
2. proposed flag name (e.g. `--vasp`)
3. Instructions how to read the potential file into a 3D mesh
4. Instructions how to read the cell from the potential file
5. units used for lattice vectors (Å vs. bohr) and potentials (eV vs. Hartree vs. Rydberg)
6. Example potential files (1 defect, 1 reference)
7. Optional: instructions for reading atomic positions

Instructions how to interpret the file can be given in written, or in form of an example code, preferentially C, C++. (FORTRAN90 or higher is OK, FORTRAN77 is not – I am too young to know this). Point 7 is needed if you want support for the atomic sphere averages. I like to emphasize that the tone of a request is important, see the excellent notes by Clint Whaley from the ATLAS package: <http://math-atlas.sourceforge.net/faq.html#utone>.

For testing purposes, a non-cubic cell with different mesh dimensions along the first and last direction will help to detect problems with mesh order. A non-symmetric orientation of the cell ($a_y^1 \neq a_x^2$), e.g. a hexagonal cell with a_1 parallel to the x-axis, will help to detect transpose mistakes in reading the lattice vectors. Telling me the charge and the dielectric constant (approximately) will help to detect problems with the units.

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