

Please post your questions for Dr. Martijn Marsman here:

Q: Why is the Wannier90-VASP interphase not working for the new versions of wannier90?

A: The API of Wannier90 was changed from Wannier90-1.2 to Wannier90-2.X. To compile VASP with Wannier90-1.2 one needs to set the pre-compiler option `-DASP2WANNIER90`, for compilation with Wannier90-2.X one needs to specify `-DASP2WANNIER90v2`.

Unfortunately, not only the API (arguments of Wannier90 in library mode) changed. In addition the way spinors (non-collinear magnetism) are treated changed from Wannier90-1.2 and Wannier90-2.X. This is broken in the interface to Wannier90-2.X.

We now have repaired this and have upgraded our interface to work with Wannier90-3.X.

This will be part of the upcoming release of VASP.6.2.X.

As of that time we will only support interfacing to Wannier90-3.X (and beyond hopefully).

Q: Are there known problems currently with the HSE06 hybrid functional interfacing with Cori KNL nodes (for newer versions of VASP) ?

A: Since you ask, I infer there might be ... but I'm not aware of any.

Q. How does the RPA compare with hybrids for computational time?

A: Roughly 10 times slower.

Q. Are SIC obsolete now? It was argued lately that SIE is responsible for the wrong CO adsorption site.

A: I am not aware of substantial new work on self-interaction corrections (the last I know Nicola Marzari was working on it some years ago, but I do not know what came of that particular development).

Q: How does the RPA compute the excited state?

A: By solving the GW quasi-particle equations. The energies of the "occupied" quasi-particle states correspond to the energy it cost to remove an electron (in that state) from the system, and quasi-particle energies of the occupied states correspond to the energy gained by adding an electron to the system in that particular state.

Q. Will any future versions of VASP support interactive structure updates? This would greatly enhance the capabilities of packages like Pymatgen and ASE to use VASP as a back-end.

A: This is already possible in principle, but not actively supported as yet. It is a good point. I will look into this in detail asap.

Q: In cases where memory becomes a significant problem, is it best to go back to the older, slower ACFDT algorithm, or experiment with reducing the size of the frequency grid? What approaches would you recommend?

A: I would advocate going to more nodes. The memory demand of the cubic scaling ACFDT algorithm is large, but it is distributed.

Q: How does the RPA work for 3d transition metals since the implementation is perturbative?

A: We do not have extensive experience (yet). The RPA is not expected to be great for the description of strong correlation where the groundstate is expected to be of a multi-determinantal nature.

Q: Is there a self-consistent version of this RPA correlation?

A: The total energy functional that corresponds to self-consistent GW is the Luttinger-Ward functional, while for single-shot calculations the Klein-functional should be used and results in the logarithmic formula that we call ACFDT/RPA as shown in the presentation. We generally propose to perform single shot RPA calculations on top of PBE or other GGA calculations.

Q: Can the ACFDT formalism be used to calculate optical excitation lifetimes? If yes, is there any plan to add this functionality to VASP in the future?

A: No, one can compute the lifetimes of the GW quasi-particle, but for optical excitations you'd need the lifetimes of electron-hole pairs, right? These kind of excitations require something like BSE. VASP can do BSE calculations (very expensive) but for the moment does not compute lifetimes, only spectra.

Q: Can you say a few words about forces in RPA?

A: In contrast to the normal situation in the RPA the orbitals are not self-consistent (w.r.t. the total energy functional). This gives rise to non-Hellmann-Feynman contributions to the forces. In practice this means that to compute the RPA forces VASP has to do an additional linear response calculation.

Q: When will HDF5 support be added to VASP 6? (Q: from a different person, I'm assuming this question is about storing of volumetric data, we have also noticed that AECCAR and ELFCAR are reported to a different precision than CHGCAR which can cause issues, could a HDF5 format help unify how these are stored?)

A: We are currently actively working on the HDF5 support in VASP. The upcoming release version (6.2.0) should have something useable, but it will be a while before all possible output is ported to HDF5 as well. We are also working on a library of python functions that will facilitate reading and post-processing the HDF5 output.

Q: Can you relax the structure with RPA in VASP 6 (e.g. IBRION=0,1,2, ISIF=2/3/...)? Is RPA relaxation much slower than RPA total energy calculation? How does that compare with GGA and hybrids (computational time)?

A: Yes one can relax structures in the RPA in the manner you mention. This is quite a bit slower than doing single point RPA total energy calculations since computing the RPA forces involves an additional linear response calculation.

Q: What about accuracy in transition-state energies/activation energies for reactions?

A: We do not really know yet, but barriers are bound to be difficult because the wave function at the transition state is often of a multi-determinantal nature. This means the RPA will not necessarily be great.

Q: have you computed charge transfer for the case of CO/Pt(111)?

A: No.

Q: Can the new version vasp calculate the excitation of electrons and can we define a certain electron excited from one certain atom in the system?

A: Excited states can be described for instance by solving the GW quasi-particle equations. The quasi-particle states, like Bloch states, in principle extend over the whole system. One can not generally attribute an electron to a particular atom, and hence one can not "excite" it either.

Q: To what extent do the RPA results depend on choice of functional for initial DFT step? e.g. PBE vs PBEsol etc.?

A: I do not have a lot of data on this. We tend to stick to PBE. On one of the slides of the presentation (about C6 coefficients for noble gas solids) there are RPA results based on LDA and PBE. The effect is noticeable but not overly large.

Q: When using a different functional eg PBEsol, does it matter physically or practically that the VASP POTCARs are optimized for PBE? I have had conflicting answers to this question and haven't been able to find a good reference

A: We expect the transferability of the PAW potentials to be high enough so that using a POTCAR that was generated for PBE with a different functional (e.g. PBEsol) should not be a problem.

Q: It was mentioned to use HSE to calculate the DFT wavefunction before RPA in cases where PBE DFT gives badly wrong eigenenergies (eg predicting metallic), is it ok to use a Hubbard +U here instead of HSE?

A: Yes, that is a possibility as well.

Q: Because the implementation of RPA in the latest version scales as $O(N^3)$ and in older versions as $O(N^4)$, can we expect to get the same absolute energies with RPA in the latest version and the older version of VASP?

A: All other parameters being equal, yes. The computational complexity of the algorithm does not determine the result.

Q: Related to the above question, in general, can we expect to get the same absolute energies with GGAs and meta-GGAs in different versions of VASP when the same input file is used in different versions?

A: Yes, this should be the case. Sometimes, however, bugs get fixed, or defaults are changed that affect the absolute values of the energies. This happens rarely and we try to avoid it as much as possible so as not to break compatibility.

Q. Are there any plans to add support for automatic generation of generalized regular k-point grids in VASP?

A: Yes, we are looking at the possibility to integrate this in VASP.

Q: What is the memory scaling of RPA?

A: The storage demands scale quadratically with system size.