

# Development of first principles electronic-structure calculation software by combining effective-model derivation code RESPACK and model-analysis codes $\mathcal{H}\Phi$ and mVMC

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As Project for advancement of software usability in materials science at the fiscal year of 2018, we have released a new version of the software RESPACK [1] for many-body perturbation calculation and effective low-energy model derivation. RESPACK is possible to derive parameters for the effective low-energy model from first principles. The new version includes *ab initio* GW calculation and utility tool such as transfer analysis and interfaces to model-analysis solvers mVMC [2] and  $\mathcal{H}\Phi$  [3]. Users can now automatically obtain the model-analysis-software inputs via RESPACK.

RESPACK consists of five programs:

- Wannier function calculation (`wannier`)
- Dielectric function calculation (`chiqw`)
- Electronic interaction calculation for direct and exchange integrals (`calc_w3d`, `calc_j3d`),
- *Ab initio* GW calculation (`calc_gw`),
- Utility code for transfer analysis (`transfer_analysis`)

These programs are run under the following inputs:

- Input file for RESPACK calculation (`input.in`)

- Band-calculation outputs contained in a directory `dir-wfn`

RESPACK supports *ab initio* band calculation codes using norm conserving pseudopotentials plus plane wave basis set, and officially supports xTAPP [4] and QUANTUM ESPRESSO [5] packages. Automatic generation scripts which convert results of the band calculation to inputs for RESPACK is prepared for xTAPP and QUANTUM ESPRESSO codes. An input file for specifying RESPACK calculation conditions is designed pursuing simplicity and is given in a namelist format. It supports OpenMP/MPI and can be used in both laboratory-computer environment and System B at ISSP, the University of Tokyo. RESPACK has a wide application including simple metals, semiconductors, *3d/4d* transition-metal compounds, organic and aromatic compounds, etc. In this report, we present an *ab initio* calculation of the excitation spectrum of an impurity system using three software: xTAPP, RESPACK, and  $\mathcal{H}\Phi$ .

Figure 1(a) is the atomic geometry of the impurity system of ruby ( $\text{Al}_2\text{O}_3:\text{Cr}$ ), and the panel (b) is our calculated band structure, where we see two impurity bands near the Fermi level due to the Cr impurity. Blue dotted curves are the Wannier interpolated band

obtained from `wannier` program. We also performed `chiqw`, `calc.w3d`, and `calc.j3d` and calculated effective interactions.

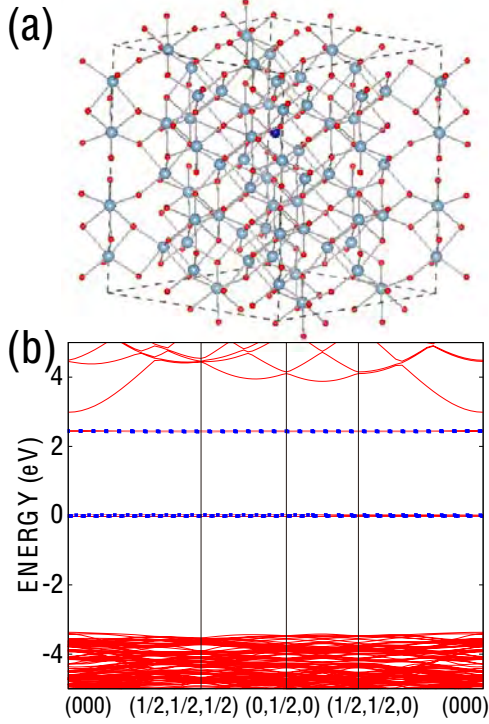


Figure 1: (a) Atomic geometry for impurity system: Al<sub>47</sub>CrO<sub>72</sub> (2×2×1 supercell). (b) Calculated xTAPP band structure with 5×5×5  $k$ -point sampling and 100-Ry cutoff.

When the RESPACK job (`wannier`, `chiqw`, `calc.w3d`, `calc.j3d`) is executed, a directory `dir-mvmc` is generated under the calculation directory, and the files necessary for model-analysis softwares mVMC and  $\mathcal{H}\Phi$  are output. Using these data and a standard-mode input for mVMC and  $\mathcal{H}\Phi$ , all inputs of the model calculations are automatically generated under the following command:

```
HPhi -s stan.in (or vmc.out -s stan.in)
```

Here, `HPhi` and `vmc.out` are execution files of  $\mathcal{H}\Phi$  and mVMC, respectively, and `stan.in` is an input file for standard mode. This interface code has the lattice conversion function; when the user moves from *ab initio* calculation to model one, the lattice adopted at the *ab initio* calculation can be flexibly changed. Also, the code has an option for avoiding the Hartree-term double count; user can adjust one-body

correction  $\Delta_{i0}$  by optional parameter  $\alpha$ ,

$$\begin{aligned} \Delta_{i0} = & \alpha U_{i0,i0} D_{i0,i0}^{\text{KS}} \\ & + \sum_{\mathbf{R} \neq \mathbf{0}} \sum_k D_{k0,k0}^{\text{KS}} \left( U_{i0,k\mathbf{R}} - (1 - \alpha) J_{i0,k\mathbf{R}} \right), \end{aligned} \quad (1)$$

where  $U$ ,  $J$ , and  $D$  are the direct integral, exchange integrals, and density matrix with the Kohn-Sham orbital, respectively.

Table 1 shows our calculated excitation energy diagram of the impurity model. The excitation energy depends on  $\alpha$  in Eq. (1), and the results correcting of the Hartree-term double counting reasonably reproduce the experimental result.

Table 1: Calculated energy diagram of impurity model from RESPACK. The unit is eV. Values of the ground state (GS) are the total energy.

Expt	Theory		
	$\Delta_{i0} = 0$	$\alpha = 0.5$	$\alpha = 1$
-			
GS( <sup>4</sup> A)	47.9( <sup>4</sup> A)	5.60( <sup>4</sup> A)	-3.04( <sup>4</sup> A)
1.79( <sup>2</sup> E)	1.67( <sup>2</sup> E)	1.61( <sup>2</sup> E)	1.62( <sup>2</sup> E)
1.87( <sup>2</sup> T)	1.78( <sup>2</sup> T)	1.73( <sup>2</sup> T)	1.84( <sup>2</sup> T)
2.23( <sup>4</sup> T)	2.29( <sup>4</sup> T)	1.79( <sup>4</sup> E)	2.32( <sup>2</sup> A)
2.62( <sup>2</sup> T)	2.46( <sup>4</sup> T)	2.23( <sup>4</sup> T)	2.56( <sup>4</sup> T)
3.10( <sup>4</sup> T)	2.69( <sup>2</sup> T)	2.60( <sup>4</sup> A)	2.78( <sup>4</sup> T)

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## References

- [1] <https://sites.google.com/view/kazuma7k6r>
- [2] <https://github.com/issp-center-dev/mVMC>
- [3] <http://issp-center-dev.github.io/HPhi/index.html>
- [4] <http://xtapp.cp.is.s.u-tokyo.ac.jp/>
- [5] <http://www.quantum-espresso.org/>