Corvus: A Workflow Tool for X-Ray and Related Spectroscopies

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Great strides have been made over the past decade in the theory and calculation of X-ray and related spectra. Some advances involve predictions of material properties such as structure or dynamics in order to make a prediction more complete, thus requiring less input, or otherwise reducing the number of free parameters required to fit to experimental data. Other advances, e.g., GW/BSE approaches, improve common approximations for electron correlation or electron-phonon interactions. However, many of these advanced methods require a combination of approaches to obtain complete calculations. Thus users must be proficient in a variety of codes, with multiple input and output formats. Moreover, users must usually manually link codes by translating the output of one to a format consistent with the input of the next. These aspects of state-of-the-art approaches create barriers to their widespread use and hence reduce the overall quality of theory and analysis methods for X-ray spectra.

To address this situation we present Corvus [1], a property driven workflow tool designed to combine and execute multiple codes. Corvus interfaces electronic structure, molecular or crystal structure, and molecular dynamics or phonon effects, with end-product codes for calculating spectroscopic quantities such as XAS. Thus Corvus serves to: (1) simplify and unify input and output formats; and (2) automatically create workflows based on target properties and input supplied by a user. The simplification of input/output works through a set of code-specific translation routines to eliminate the need for users to learn a multitude of formats, while automating the translation of output to be used in the next step in the workflow chain. The automatic generation of workflows sets up a dependency tree for target properties, which can be filled by user input, online database search, or calculations. This allows users to focus on physical properties of interest, rather than on details of any one calculation step. At present, translation tools exist for several DFT and MD codes as well as spectroscopy codes. More capabilities will be added as implementation of new code interfaces is relatively easy.

We have applied Corvus to a variety of workflows, for example: structural optimization with ORCA [3], followed by calculations of XES and RXES using FEFF [2]; DFT/MD averaged XANES using NWCHEM [4] and FEFF; and FEFF calculations of XAS using *ab initio* Debye-Waller factors obtained from dynamical matrices provided by ABINIT [5]. Examples of Corvus simplified input, and automatically generated workflows are presented, together with results that yield improved agreement in comparison to experiment.

[1] S. Story, Thesis, http://hdl.handle.net/1773/34136 (2015);
[2] J.J. Rehr et al., Phys. Chem. Chem. Phys., **12**, 5503-5513 (2010)
[3] F. Neese, Wiley Interdiscip. Rev. Comput. Mol. Sci. **2,** 73-78 (2012)
[4] M. Valiev et al., Comput. Phys. Commun. **181**, 1477 (2010)
[5] X. Gonze et al., Comput. Phys. Commun. **180**, 2582-2615 (2009)

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