Abstract Submitted
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Automated, ab initio calculations of X-ray spectra including many-body excitations and vibrational damping[1] KEVIN JORISSEN, SHAUNA STORY, JOHN REHR, Univ of Washington — Accurate calculations of x-ray absorption spectra (XAS) often require linking several materials science codes [1]. To reduce the complexity and support the hardware requirements of such calculations, we have virtualized XAS modeling workflows using a Cloud-based approach, with interfacing and configuration of codes handled by developers, and virtual HPC resources allocated on demand [2]. When coupled to user-friendly GUIs this puts powerful multi-code simulations in the hands of general users. For instance, FEFF users can improve XAS interpretation and analysis using accurate ab initio Debye-Waller factors and self energy from the ABINIT DFT code, rather than semi-empirical models. Additionally, such workflows allow robust automation of large-scale calculation sets such as the Materials Project [3] where our approach could enable a theoretical spectroscopy database of many thousands of structures for systematic study of materials.

[1] Rehr et al., C.R. Phys. 10, 548 (2009).
[2] Jorissen et al., Comp. Phys. Comm. 183, 1922 (2012).
[3] www.materialsproject.org

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