

# X-ray Raman scattering calculations with the OCEAN code

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Many X-ray absorption events can be described accurately within a two-particle framework that accounts for the explicit interactions between the excited electron and the core-hole, as well as an averaged interaction of each particle with the rest of the system. Formally, this amounts to evaluating ladder diagrams and requires solving the Bethe-Salpeter equation. Contrary to common assumption, obtaining X-ray spectra through the Bethe-Salpeter equation is actually quite computationally efficient as it does not require use of supercells, eliminates summations over final states, and allows for a real-space evaluation of the core-hole screening response. I will present the implementation of the Bethe-Salpeter equation within the OCEAN code [1] as it pertains to X-ray Raman scattering and will provide a brief description of the use of the code. Several recent scientific use cases will be presented [2-4]. I will conclude with some thoughts on including additional many-body effects and prospects for applications on strongly correlated materials.

## References

- [1] - K. Gilmore *et al.*, *Computer Physics Communications* **197**, 109 (2015).
- [2] - J. Niskanen *et al.*, *Physical Review E* **96**, 013319 (2017).
- [3] - S. Petitgirard *et al.*, *Geochemical Perspectives Letters* **9**, 32 (2019).
- [4] - G. Spiekermann *et al.*, *Physical Review X* **9**, 011025 (2019).