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Response theory techniques to address X-ray spectroscopies

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With the installation of the fourth-generation synchrotron facility MAX IV in Sweden and XFEL facilities around the world, the Knut and Alice Wallenberg Foundation has initiated a concomitant investment in the development of theory and simulation techniques. The resulting Consortium for Theoretical X-ray Sciences (CoTXS) initiative builds on the active collaboration and synergy between seven leading theoretical groups in Sweden with principal investigators P. Norman, I. Abrikosov, R. Lindh, O. Eriksson, L.G.M. Pettersson, Y. Luo, and H. Ågren.

We will present recent advances in response theory, designed to address molecular systems under electronic resonance conditions and referred to as the complex polarization propagator (CPP) approach [1]. In the CPP formulation, electronic relaxation in the core-excited state becomes a matter of electron correlation as illustrated in studies employing the hierarchical sets of coupled cluster (CC) and algebraic diagrammatic construction (ADC) methods. The full propagator formulation of inelastic scattering matrix elements (the Kramer–Heisenberg–Dirac formula) has been derived in the ADC framework, which provides a response theory treatment of resonant inelastic X-ray scattering (RIXS) spectroscopy [2]. The CPP approach is open-ended for extensions toward nonlinear X-ray spectroscopies [3], such as e.g. X-ray two-photon absorption (XTPA) [4], which are of concern in connection with research at X-ray free electron laser (XFEL) facilities.

[1] Norman, P., Ruud, K., Saue, T. (2018). Principles and Practices of Molecular Properties. Chichester, UK: John Wiley & Sons, Ltd. http://doi.org/10.1002/9781118794821

[2] Rehn, D. R., Dreuw, A., Norman, P. (2017). Resonant Inelastic X-ray Scattering Amplitudes and Cross Sections in the Algebraic Diagrammatic Construction/Intermediate State Representation (ADC/ISR) Approach. Journal of Chemical Theory and Computation, 13(11), 5552–5559. http://doi.org/10.1021/acs.jctc.7b00636

[3] Fahleson, T., Norman, P. (2017). Resonant-convergent second-order nonlinear response functions at the levels of Hartree–Fock and Kohn–Sham density functional theory. The Journal of Chemical Physics, 147(14), 144109. http://doi.org/10.1063/1.4991616

[4] Fahleson, T., Ågren, H., Norman, P. (2016). A Polarization Propagator for Nonlinear X-ray Spectroscopies. The Journal of Physical Chemistry Letters, 7(11), 1991–1995. http://doi.org/10.1021/acs.jpclett.6b00750

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