# Simulating X-ray Photoelectron Spectra of Solids Using Periodic Algebraic Diagrammatic Construction Theory

Abdelrahman Ahmed[†], Alexander Yu. Sokolov
Department of Chemistry and Biochemistry,
The Ohio State University, Columbus, OH, 43210
[†]E-mail: ahmed.796@osu.edu

With its sensitivity to local chemical environments, core-level x-ray photoelectron spectroscopy (XPS) is a powerful tool for a variety of applications, ranging from quantifying the composition of surfaces to elucidating the electronic structure of matter. However, the assignment and interpretation of experimental XPS spectra that probe core-level electrons is often difficult, necessitating employing accurate, yet computationally efficient methods to simulate spectra reliably. Developing such methods, however, is not straightforward. Some challenges include choosing basis sets of appropriate size and type, and faithfully describing the strong orbital relaxation that results from the creation of a core-hole on top of dynamical electron correlation effects. While several methods have been developed for the simulation of core-level XPS, they either incur a high computational cost, or provide an inadequate description of the aforementioned physical effects. In this work, we have combined the core-valence separation (CVS) approximation with our recent implementation of periodic algebraic diagrammatic construction (ADC) theory, to accurately and reliably simulate core-level XPS spectra of solids. By leveraging the power of perturbation theory, ADC offers a relatively low-cost, systematically improvable framework that accurately incorporates orbital relaxation and electron correlation effects, while combining it with CVS allows us to access the x-ray spectral window. We will present a benchmark of periodic CVS-ADC by calculating ionization energies of different edges (e.g. K-, and L-edges) for a variety of systems, such as diamond, Aluminum Phosphide, and Zinc Oxide. Further, we will demonstrate that periodic CVS-ADC energies are in excellent agreement with experiment when extrapolated to the thermodynamic limit. Lastly, we will show results of simulated XPS spectra of materials, such as Boron Nitride and Titanium Dioxide, and discuss how our method is able to reproduce important spectral features, such as satellite peaks and accurate peak spacings.