Abstract Submitted
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A Many-Body Formalism of ΔSCF Approach for Simulating X-Ray Spectra from First-Principles[1] YUFENG LIANG, The Molecular Foundry, Lawrence Berkeley National Laboratory (LBNL), JOHN VINSON, National Institute of Standards and Technology (NIST) , SRI PEMMARAJU, The Molecular Foundry, Lawrence Berkeley National Laboratory (LBNL), WALTER DRISDELL, Chemical Sciences Division, Lawrence Berkeley National Laboratory (LBNL), ERIC SHIRLEY, National Institute of Standards and Technology (NIST), DAVID PRENDEGAST, The Molecular Foundry, Lawrence Berkeley National Laboratory (LBNL)
— Accurately reproducing X-ray spectral fingerprints for materials characterization relies heavily on how to correctly model the many-electron response to the generation of an X-ray core hole. In this talk, we present a novel first-principles theory for simulating X-ray spectra that is based on many-electron wavefunctions. The proposed theory go beyond the electron-hole correlations within the Bethe-Saltpeter Equation and consider higher-order vertex corrections up to the level of Mahan-Noziéres-De Dominicis (MND) theory. An efficient algorithm is invented to incorporate these many-electron processes by using linear algebra rather than iterating over all Feynman diag

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