## Conference on Quantum-Many-Body Correlations in memory of Peter Schuck (QMBC 2023)



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## Core level chemical shift by ab initio mehods: from mean-field to many-body theory

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The binding energy of core electrons may not only provide information on the chemical composition, but also some additional information such as the type of bonding, which could be inferred from the shift of the binding energy, (also known as chemical shift). We present the study of the chemical shift using different theories, from Hartree-Fock and density-functional theory to many-body perturbation theory (COHSEX, *GW*). We benchmarked the accuracy of the chemical shift of the carbon 1s electron in a set of molecules against experiments. Besides, our study reveals the physical origin of the chemical shift.

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