

# Ab Initio Self-Consistent GW+EDMFT for Quantum Materials

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Accurate first-principles descriptions of correlated quantum materials require a simultaneous treatment of strong electronic correlations and screening effects. Fully self-consistent GW+EDMFT provides a natural framework for this purpose by combining nonlocal correlation effects at the GW level with local vertex corrections from extended dynamical mean-field theory (EDMFT). Applying this framework to realistic materials, however, remains computationally demanding because of the cost of evaluating two-particle correlation functions with full frequency dependence and iterating self-consistently over both the Green's function and screened interaction.

In this talk, I will present recent developments in CoQuí, a software platform for ab initio many-body electronic-structure calculations [1,2]. Central to CoQuí are interpolative separable density fitting and compact imaginary-axis representations of correlation functions. These techniques reduce computational costs across a range of many-body approximations.

As representative applications, I will present fully self-consistent GW+EDMFT calculations for transition-metal oxides [3], spanning band insulators, Mott insulators, and correlated metals. These calculations use no empirically fitted interaction parameters and yield electronic properties in good agreement with experiment. I will discuss how self-consistency changes screening and electronic structure, and compare how local vertex corrections affect screened interactions, self-energies, and spectral properties from one material to another.

[1] C.-N. Yeh and M. A. Morales, *J. Chem. Theory Comput.* **19**, 6197–6207 (2023).

[2] C.-N. Yeh and M. A. Morales, *J. Chem. Theory Comput.* **20**, 3184–3198 (2024).

[3] C.-N. Yeh, F. Petocchi, A. Hampel, P. Werner, O. Parcollet, A. Georges, and M. A. Morales, *arXiv:2603.12336* (2026).