The density is not enough

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Density-functional theory is a powerful and widely used tool for materials simulations, thanks not only to its accuracy, but also the simplicity of having a functional formulation.

However, in its current approximations it does not entirely fulfill the needs for qualitative or quantitative accuracy in the prediction of materials' properties. More importantly, it also suffers from a foundational limit - as a functional theory of the total electronic density, it is unable to predict even in principle single-particle energy levels. Thus, one is forced to devise energy functionals that aim at accuracy while remaining unaware of what the true energy levels should be (the highest-occupied one being the exception, at least in exact DFT).

Driven by efforts in correcting qualitative failures of common DFT approximations, I'll discuss our suggestion of enforcing a generalized Koooopmans' condition to energy functionals, illustrating both the features of the resulting beyond-DFT framework, and its accuracy in predicting e.g. photoemission spectra. More broadly, I'll argue how this formulation points towards more general functional theories able to reproduce simultaneously both total energies and spectral properties.