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Some thoughts about old and new density functionals

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The only theoretical approximation that lies at the heart of DFT appears is the (in)famous exchange-correlation functional. It is therefore not surprising that this quantity has been extensively studied, and that more than 150 different approximations have been put forward in the past 50 years. In this talk I will show some results concerning different families of functionals. The first concerns hybrid functionals, and in particular the role of the mixing parameter. This is commonly assumed to be fixed at a value around 0.2-0.3. However, by noting the similarities between the hybrid functionals and screened Hartree-Fock and ultimately GW theories, we can relate this parameter to the screening properties of the system. In this way we can build a recipe that allows for a considerable improvement on the results obtained by traditional hybrid functionals for solids. As a second topic, I will discuss if it is possible to completely get rid of the Slater integrals present in both Hartree-Fock, hybrid functionals or OEP approaches, and anyway get a proper description of the exchange in terms of reduced densities. I will pay particular attention to the new meta-GGA functionals for the exchange potentials, like, e.g., the Becke-Johnson potential and its more recent variations, like the Tran and Blaha or the Rasanen, Pittalis, and Proetto functionals.