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New models for mixing wavefunctions with density functional theory

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The recent realization that the ground-state correlation energy of the random phase approximation (RPA) is intimately connected to an approximate coupled cluster doubles (CCD) model [1], opens interesting avenues for mixing RPA with DFT [2]. I will also present a new constrained-pairing mean-field theory (CPMFT) that describes strong correlations quite accurately [3,4]. Dynamical correlation functionals for this model are feasible but they require the use of "alternative" densities.

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