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Strong correlation in Kohn-Sham DFT[1] FRANCESC MALET GIRALT, ANDRÉ MIRTSCHINK, Vrije Univ (Free Univ), JONAS CREMON, Lund University, CHRISTIAN MENDL, Technische Universität München, KLAAS GIESBERTZ, Vrije Univ (Free Univ), STEPHANIE REIMANN, Lund University, PAOLA GORI-GIORGI, Vrije Univ (Free Univ), MATHEMATICAL PHYSICS, LUND UNIVERSITY COLLABORATION, MATHEMATICS DEPARTMENT, TECHNISCHE UNIVERSITÄT MÜNCHEN COLLABORATION — The knowledge on the strong-interacting limit of density functional theory can be used to construct exchange- correlation functionals able to address strongly-correlated systems without introducing any symmetry breaking. We report calculations on semiconductor nanostructures and one-dimensional models for chemical systems, showing that this approach yields quantitatively good results in both the weakly- and the strongly-correlated regimes, with a numerical cost much lower than the traditional wavefunction methods.

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