

Abstract Submitted
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Total and self-energies beyond LDA and GGA: exact-exchange, GW and MP2 united by numeric atom-centered orbitals XINGUO REN, ANDREA SANFILIPPO, ALEXANDRE TKATCHENKO, Fritz Haber Institute, Berlin, Germany, PATRICK RINKE, University of California at Santa Barbara, CA, VOLKER BLUM, KARSTEN REUTER, MATTHIAS SCHEFFLER, Fritz Haber Institute, Berlin, Germany — Well-known deficiencies of (semi-)local exchange correlation functionals in density functional theory comprise the spurious self-interaction, the absence of long-range correlation, and the absence of the derivative discontinuity with respect to the electron number. Present approaches to overcome these deficiencies (e.g., hybrid functionals, MP2, and GW) typically involve expensive two-electron Coulomb repulsion integrals. For molecules, the resulting numerical effort usually restricts these methods to Gaussian basis functions. We here show how all these methods can be handled accurately with efficient all-electron numerical atom-centered basis sets [1], by using a second, auxiliary basis for products of basis functions (resolution of the identity). For an extended set of finite systems spanning small molecules (water dimer, benzene), metal clusters (Na_n) and biomolecules (polyalanine peptides), we demonstrate that the efficiency of optimized numeric atom-centered basis sets is directly carried over into our new approach. Our approach is then applied to analyze the CO-adsorption problem (CO/Cu(111)). [1] V. Blum *et al.*, The FHI-aims project, www.fhi-berlin.mpg.de/aims

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