Accuracy tests of EXX+RPA scheme in r-space implementation of KS-DFT

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In this communications, we present technical details of the implementation of the exact-exchange (EXX) [1] contribution to the Kohn-Sham potential, with correlation energy calculated employing the random phase approximations (RPA), which have proved to account for correct description of the Van der Waals interactions [2]. This implementation is done on the newly developed code in our group, in which the Kohn-Sham equations [3] are directly solved on a grid in the r-space. Calculations in r-space, in contrast to the majority of available commercial and under GNU license available computer codes, allows for employing the periodic boundary conditions only along physically periodic directions, i.e., without the necessity of placing partly periodic systems into an artificial three-dimensional super-cell. This allows for more efficient computations of the electronic properties.

In order to check the efficiency (computational burden, time consuming) and the accuracy of our real space code, we study representative systems of carbon-based materials, in which the Van der Waals interactions are of particular importance, such as graphite; bi- and tri-monolayers of graphene, carbon nanotubes, and simple molecules C_2. These systems exhibit different types of periodicity, therefore, we also compare the obtained results with the ones obtained within standard supercell calculations. Moreover, in all of these cases we examine the accuracy of the pseudopotential EXX scheme with the all electron approach (commercial all-electron code FHI-aims [4]), by comparing the structural and electronic properties of representative systems.

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