O.12 New features related to the exchange and correlation functionals in ABINIT

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Since the last ABINIT developer workshop, we have extended the ABINIT capabilities related to the electronic exchange and correlation processing in ABINIT.

Concerning ground state calculations, first, we have introduced the possibility to use meta-GGA XC functionals including the core electrons contribution. On the other hand, we have made possible the meta-GGA calculations in the PAW formalism. This required a small adaptation of the ATOMPAW atomic dataset generator. It was also necessary to derive formulas for the calculation of the stress tensor. We present results obtained on hydrides using the SCAN functional and compare them to GGA calculations.

Concerning the response function calculations, we have derived the equations to perform Raman intensity calculations in the Genelarized Gradient Approximation (GGA), both for norm-conserving pseudo-potentials and for the PAW approach, and specifically in the DFPT formalism. For this, we used the latest features of the libXC library in its version 5. The correponding formulas are quite long and require a rather complex test procedure. In this perspective, we have developed a numerical test module for the validation of exchange-correlation contributions to the energy and its derivatives up to order 3.