O.13 Updates to the atomic dataset generator program ATOMPAW

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In collaboration with Marc Torrent (CEA) and Michel Côté (U. Montréal) a number of updates to the ATOMPAW code have been introduced. Ongoing progress on the effort to develop self-consistent PAW (Projector Augmented Wave [1]) datasets for the meta-gga formalism will be presented. In particular, within the context of the generalized Kohn-Sham formalism, the functional dependence on the kinetic energy density alters the form of the Kohn-Sham differential equations and introduces some numerical challenges. Preliminary results for a slightly modified version of the r^{2}SCAN functional [2] appear to be promising.

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[1] P. Blöchl, *Phys. Rev. B* **50** 17953-17979 (1994)

[2] J. W. Furness, A. D. Kaplan, J. Ning, J. P. Perdew, and J. Sun, *J. Phys. Chem. Lett.* **11**, 8202-8215 (2020)

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