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Trying different xc functionals for warm dense matter

Tuesday 22 February 2022 14:30 (30 minutes)

Libxc, one of a few available libraries for exchange-correlation functionals, currently contains well above 100 different LDA, GGA, hybrid GGA, meta-GGA, and hybrid meta-GGA functionals. The aim of this talk is to show the results of trying quite a few of these for different warm dense matter states and different properties. When possible, quantum Monte Carlo data will be used to benchmark the DFT results.

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