

Double Hybrids for the Solid State by Local Correlation Methods

LORENZO MASCHIO¹, FABIO DELLA SALA², EDUARDO FABIANO² and
BARTOLOMEO CIVALLERI¹

¹*University of Torino, Via Pietro Giuria 5, Torino, Italy*

lorenzo.maschio@unito.it

²*CNR-IMM, Via Monteroni, Lecce, Italy*

ABSTRACT

Double hybrid functionals are a well-known approach for climbing Jacob's ladder. Despite that, their development and application in the framework of ab initio simulation of crystalline solids sort of lags behind.

In this contribution we will present our approach based on local-correlation methods for the solid state.[1,2] Benchmarks will be shown for several functional recipes, including XYG3 [3] and the recent Adiabatic-Connection models which interpolates towards the strong-correlation limit. [4]

References

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