Recent developments in local correlation methods for solids.

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Abstract

Local correlation methods [1,2] adapted for crystalline periodic systems [3-5] have been demonstrated to be a powerful tool for the accurate post-HF study of solids [6-9], also thanks to the implementation of specific density-fitting techniques [10].

In this contribution I will report on the most recent advances, including the implementation of Orbital-Specific Virtuals [11] in our periodic Local-MP2 program, and benchmarking of range-separated DFT/LMP2 methods for describing dispersive interactions in crystals.[12]

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