

[L4] Localized Views on Delocalized Systems: A Risky Acrobatics?

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Traditionally, periodic systems are examined using the elegant Bloch's theorem, introducing the concept of reciprocal space. Another strategy would be to start from elementary building blocks and their electronic structure to reconstruct the full system [1]. This is the route we followed to explore the ground state energies and charge gap in low dimensional extended systems. The method will be exemplified based on model Hamiltonians.

Bibliography:

[1] M. Kepenekian, V. Robert, C. Boilleau, J.-P. Malrieu Phys. Chem. Chem. Phys. 14 (2012) 138