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

Vincent Robert¹, Mikael Képénékian², Jean-Paul Malrieu³

¹Laboratoire de Chimie Quantique, Université de Strasbourg/Institut de Chimie, 4 rue Blaise Pascal 67000 Strasbourg-FRANCE.
²Laboratoire de Chimie Inorganique Théorique, Institut de Sciences Chimiques de Rennes, campus de Beaulieu 35042 Rennes-FRANCE.
³Laboratoire de Physique et Chimie Quantique, Université de Toulouse/IRSAMC, 4 route de Narbonne 31000 Toulouse-FRANCE.

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: