Selected Molecular Systems and Their Properties from Exact Diagonalization Ab Initio Solution

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This abstract highlights our research on unraveling the intricate nature of molecular bonding by determining many-particle covalency and ionicity factors. We employ microscopic single-particle and interaction parameters within our method to calculate these factors, while also discussing their limitations. To overcome these limitations, we introduce the concept of partial atomicity, which offers a new perspective on the bonding phenomenon.

Our study addresses the challenge of accurately characterizing molecular properties and bonding behavior. By incorporating partial atomicity, we bring atomic ingredients into the collective electron states, effectively eliminating spurious behavior of covalency with increasing interatomic distance. Furthermore, this concept offers a fresh interpretation of bonding, providing a deeper understanding of the underlying physics.

The implications of our research extend to various scientific disciplines, including chemistry, materials science, and physics. By shedding light on the interplay between covalency and ionicity in molecular systems, we contribute to the development of advanced models for molecular analysis, paving the way for more accurate predictions and improved design strategies.

References:

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