Green's Function Approach to Ab Initio Band Structures of HF and HCl Chains

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Local approaches to electron correlation in atoms, molecules and solids are already very old [1]. Meanwhile, correlated ground state wave functions and energies of solids and large molecules can be obtained routinely [2] by employing Stoll's incremental scheme [3] which is a simple and robust linear scaling method that can be used in conjunction with almost any quantum chemical correlation method.

Several incremental schemes, e.g. the effective Hamiltonian approach [4], for excited states in solids have been formulated so far to establish a long sought-after method which allows to calculate correlated band structures of solids without relying on density functional theory. Another recent approach uses many-body Green's functions [5].

We propose a new Green's function approach to correlated band structures. It it based on a reformulation of the well-established algebraic diagrammatic construction scheme for localized crystal orbitals (CO-ADC). In this scheme, the band structure is obtained directly by diagonalizing a suitable matrix which incorporates all correlation effects.

We use the incremental scheme to study the ground state of the weakly bound $(HF)_\infty$ and $(HCl)_\infty$ chains. The bonding in $(HCl)_\infty$ is appreciably larger than it is in $(HF)_\infty$ leading to more delocalized orbitals and thus to a slower decay of the individual increments. Band structure calculations for $(HF)_\infty$ and $(HCl)_\infty$ are in progress.

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