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Mapping Kohn-Sham eigenenergies onto vertical ionization energies

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Abstract content
   (Max 300 words)

In Density Functional Theory the interacting system is mapped unto a fictitious independent particle model. The interpretation of the eigenenergies of the independent particle system is still an open question. In the formalism they appear as Lagrange parameters, but they may have physical content. In this presentation, it is shown that each Kohn-Sham, or independent particle eigenenergy can be mapped onto a difference between the interacting ground state energies of successive integer-electron systems via a coupling constant integration. Occupied Kohn-Sham energies can be mapped onto vertical ionization energies and virtual Kohn-Sham energies can be mapped unto vertical electron affinities. This mapping is unique for non-degenerate Kohn-Sham energies, but degenerate Kohn-Sham levels can be mapped onto multiple ionization energies or electron affinities. Exact expressions for the first ionization and electron affinity energies lead to exact formal expressions for the difference between the Kohn-Sham gap and the fundamental gap.

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