

Extracting chemical information from molecular wave functions – some recent results

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In the lecture I am going to summarize our recent results obtained for *a posteriori* analyzing molecular wave functions in chemical terms. The topics will cover

- *Bond order index*: improved definition for correlated wave functions and calculating from results of plane wave calculations;
- *Effective atomic orbitals and effective minimal basis sets*: calculations in different theoretical frameworks;
- An improved *energy-partitioning scheme*.