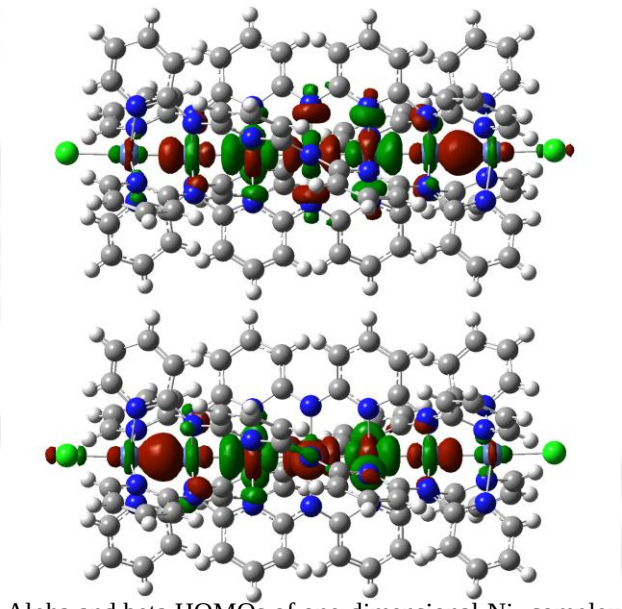
Theoretical Chemistry Colloquium

July 19, 2013 (Fri), 10:00-11:00

RCMS, 2nd floor, Chemistry Gallery

Application of a spin-projected broken-symmetry (BS) DFT to polynuclear metal complexes ~ Electronic structure, molecular structure and physical properties ~



Alpha and beta HOMOs of one-dimensional Ni_7 complex.

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Abstract: *A recent progress in quantum chemistry enables us to obtain electronic structures, molecular structures and physical properties of larger molecules by the first-principle calculations. However, a treatment of a static (non-dynamical) correlation effect on quasi-degenerate systems is still one of the difficult subjects. The broken-symmetry (BS) method approximately but easily corrects the static correlation at the lower computational cost, so that the BS DFT is now widely utilized for computational studies. In this presentation, I illustrate how the BS DFT works powerful for the polynuclear metal complexes with some calculation examples. In addition, I also show some shortcomings of this method.*

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