On the one-particle relaxation in R12/F12 theories.

Ján Šimunek,[a] Jozef Noga[a,b]

[a] *Department of Inorganic Chemistry, Faculty of Natural Sciences, Comenius University, Mlynská dolina CH2, SK-84215 Bratislava, Slovakia*

[b] *Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, SK-84536 Bratislava, Slovakia*

Abstract

When the explicitly correlated R12/F12 theories [1,2] are applied in combination with smaller one-particle orbital basis sets, the relaxation with respect to the one-particle limit basis becomes relevant.[3] Starting from a single reference Slater determinant in a given computational basis, two ways of coping with this effect are compared as to their computational complexity and the accuracy. The first approach is based on a separate expansion of single excitations using a dual Hartree-Fock limit basis, whereas the second approach is based on the full treatment of the correlation factor, including its formal one-particle component.

[1] J. Noga, W. Kutzelnigg and W. Klopper, Chem. Phys. Lett. **199**, 497 (1992).
[2] J. Noga, S. Kedžuch, J. Šimunek, and S. Ten-no, J. Chem. Phys. **128**, 174103 (2008).
[3] J. Noga, S. Kedžuch, J. Šimunek, J. Chem. Phys. **127**, 034106 (2007).