Optimized minimal atomic primitive (MAP) Slater-type basis sets

Peter Reinhardt[1], Ilya Popov[2], Andrei L. Tchougréeff[2,3]

[1] *Laboratoire de Chimie Théorique, Faculté des Sciences et de l'Ingénierie, Sorbonne Université, 4, place Jussieu, case courrier 137, F – 75252 Paris CEDEX 05, France*

email: Peter.Reinhardt@upmc.fr

[2] *Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Moscow, Russia*

[3] *Institut für Anorganische Chemie, RWTH Aachen, Landoltweg 1A, D – 52074 Aachen, Germany*

Minimal Slater basis sets have been generated for the whole periodic table, in the philosophy of having one single orbital exponent per atomic shell.[1] Minimizing the total energy for different spectroscopic states allows to extract information for generating obital lobes to project and decompose wavefunctions of solid-state applications into atom-centered contributions for describing for instance F-centers in solids, or electrides like cubic Na_2He. As well simple descriptions of bonding may be obtained for systems where one in general relies on promolecular densities or crude parametrization.

We show that fundamental properties (radial expectation values, nodal positions) of the generated orbital sets are astonishingly close to those obtained with much larger basis sets in the literature, without numerical inconsistencies due to the cancellation of exponential functions.

Possible applications, trends, and limits are discussed in this contribution.

---

[1] *I.V. Popov, A.L. Tchougréeff*, Theor.Chem.Acc, **138** (2019) online