A Software for Designing SCC-DFTB Repulsion Parameters Automatically: The Framework for Automatization of SLAKO Parameterization (FASP)

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INTRODUCTION

FASP program was developed with the aim of making the complex process of parameterizing the SCC-DFTB repulsion energy (E_{rep}) (essential for geometry and reaction energies) that involves a huge number of files, data and variables in a straightforward manner. The parameterization is fully automatic and the users only have to provide adequate references. The FASP also provides the reusability of the electronic part of the SLAKOs[1,2] available in the literature while reparameterizing the original E_{rep} for describing other systems. The results of the E_{rep} parameterization for C, H, O, N are presented. FASP will be the first tool freely available for the community that deals with the parameterization automatically.

METHODS

The SCC-DFTB energy is $E = E_{bnd} + E_{SCC} + E_{rep}$. E_{bnd} is the sum over all occupied orbital energies[2], E_{SCC} is the Self-Consistent-Charge (SCC) energy and $E_{rep}(R_{AB})$ is the repulsion energy: $E_{rep}(R_{AB}) = E_{DFT}(R_{AB}) - (E_{bnd}(R_{AB}) + E_{SCC}(R_{AB}))$(Fig. 1)[2].

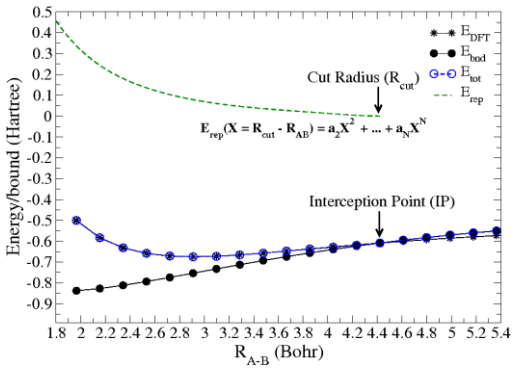

Figure 1. DFT (E_{DFT}) and SCC-DFTB (E_{bnd} + E_{SCC}) potentials and the polynomial which describes the E_{rep} all as a function of the interatomic distances (R_{AB}).

RESULTS AND DISCUSSION

Table 1 shows a comparison of the geometrical parameters for typical organic molecules and figure 1 shows a comparison of the mean error bars for 24 organic reactions with parameters obtained using different electronic part of SLAKOs.

Table 1. Bond length obtained with DFT (PBE/TZP) and SCC-DFTB (FASP, mio, matsci) approximation, all values are expressed in Å.

Property	PBE/TZP	current[a]	*mio*	*matsci*
Propyne				
C─C	1.456	1.480	1.462	1.453
C≡C	1.215	1.211	1.209	1.206
Acetic Acid				
C─C	1.506	1.533	1.499	1.511
C─O	1.373	1.398	1.385	1.447
C=O	1.217	1.227	1.213	1.216
Pyridine				
C─C	1.398	1.423	1.400	1.395
C=N	1.344	1.359	1.339	1.330
Nitric Acid				
N─O	1.449	1.449	1.419	1.332
N=O	1.222	1.234	1.208	1.235
O─H	0.984	0.978	0.998	0.974

[a] Obtained by FASP using the SLAKOs developed by Wahiduzzaman et al.[1].

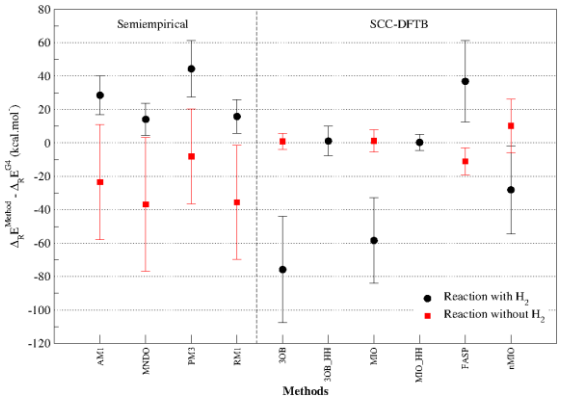

Figure 2. Description of 24 organic reactions computed by semiempirical methods and several SCC-DFTB parameters set compared to G4 method.

CONCLUSIONS

The FASP has proved to be an efficient software for developing E_{rep} parameters by taking into account both geometries and reaction energies during the automatic procedure.

ACKNOWLEDGMENTS

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[1]Wahiduzzaman et al., J. Chem. Theor. Comp., 9, 4006, (2013);
[2]Oliveira et al., J. Braz. Chem. Soc., 20, 1193, (2009);
[3]www.dftb.org.