1,3-Diketone Fluids and their Complexes with Iron

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Tribological experiments with 1,3-diketone fluids in contact with iron surfaces show ultralow friction[1], which was suggested to be connected to the formation of iron complexes. In order to support this assumption, we calculate infrared and optical spectra of various substituted 1,3-diketones and their iron complexes using gradient corrected density functional theory (DFT). The description of the complexes requires the application of the DFT+U scheme for a correct prediction of the high spin state on the central iron atom. With this approach we obtain excellent agreement between experiment and simulation in infrared and optical spectra (see fig. 1), allowing for the determination of 1,3-diketone tautomeric forms [2]. The match in the spectra of the complex strongly supports the assumption of iron complex formation by these lubricants.

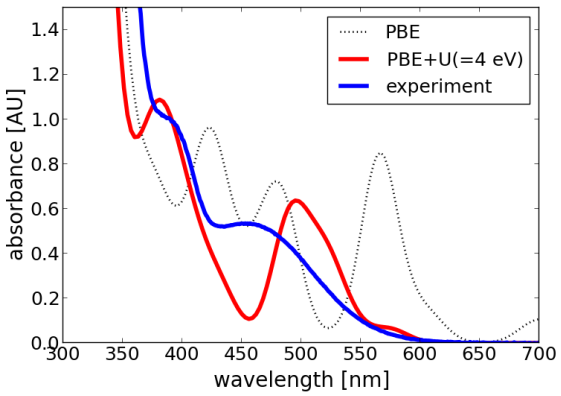

Fig. 1Comparison of simulated and experimental UV-Vis spectra.

References

[1] Amann, T., and Kailer, A. Tribology Letters 41, 2011,121–129
[2] Walter, M., Amann, T., Li, K., Kailer, A, Rühe, J., and Moseler, M. J. Phys. Chem. A, submitted 2013