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DO HYBRID FUNCTIONALS IMPROVE THE DESCRIPTION OF TM-SITES IN ZEOLITES?

A TALK BY FLORIAN GÖLTL,
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TM-exchanged zeolites are used as catalysts in the de-NO_x reaction. The reaction takes place inside the material and is everything but well understood. Direct observation using experimental methods is impossible. Therefore a reliable theoretical description is required. For TM atoms it is well known that the standard methods of Density Functional Theory (DFT) show large errors. In a series of papers we compared the performance of different hybrid functionals compared to the usual semi-local functionals within DFT[1,2,3].

Experimentally seen there are three methods used to obtain information about TM sites in zeolites. (i) XRD gives structural parameters, (ii) IR adsorption and emission spectroscopy leads to a spectrum which can be used to deduce chemical properties of the active site and (iii) the IR frequencies of adsorbed tracer molecules like CO and NO help to determine the chemical activity.

In this talk I will compare the performance of standard GGA-functionals such as PW91 and PBE to the performance of unscreened (PBE0) and screened (HSE) hybrid functionals as far as (i) structural properties, (ii) the density of states (excitation/emission spectra) and (ii) the adsorption of CO and NO in Cu(I), Cu(II) and Co(II) chabazite is concerned. Furthermore I will compare the obtained results to experiment and discuss, whether the use of computationally more demanding hybrid functionals is justified.

1 F. Göltl, J. Hafner, Structure and Properties of Metal-exchanged Zeolites Studied Using Gradient-corrected and Hybrid Functionals: I. Structure and Energetics, submitted to J. Chem. Phys.

2 F. Göltl, J. Hafner, Structure and Properties of Metal-exchanged Zeolites Studied Using Gradient-corrected and Hybrid Functionals: II. Electronic Structure and Photoluminescence Spectra, submitted to J. Chem. Phys.

3 F. Göltl, J. Hafner, Structure and Properties of Metal-exchanged Zeolites Studied Using Gradient-corrected and Hybrid Functionals: III. Energetics and Vibrational Spectroscopy of Adsorbates, submitted to J. Chem. Phys.