DENSITY FUNCTIONALS FOR CATALYSIS

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In recent years, we have developed several density functionals with broad applicability [1,2]. This lecture will present a brief summary of applications relevant to problems in catalysis. We will especially emphasize the usefulness of the Minnesota M06 and M06-L functionals.

The M06-L functional is especially interesting because of its low cost for applications to complex systems. Using the M06-L density functional, we have obtained good results for the structures of gold nanoparticles, for the energetics of zeolite binding to catalytic substrates, for the difference in the enthalpy of activation for producing first and second generation Grubbs Ru carbene catalysts for olefin metathesis, for olefin binding to Pd cross coupling-type catalysts, for the free energy of N–H bond activation by a PCP pincer complex of Ir, for a catalytic energies database, for a database of isomerization energies of large organic molecules, for noncovalent interactions, for the methyl–methyl association rate constant, for the reaction energies of water clusters and microhydrated H_3O^+ and OH^- clusters, for the thermochemistry of iron carbides, and for databases of transition metal dimer bond energies, transition-metal–ligand bond energies, and 3d transition metal reaction energies. Therefore it seems to be an excellent choice for a variety of applications involving transition metal chemistry and catalysis.

[1] Y. Zhao and D. G. Truhlar, Acc. Chem. Res. 41, 157 (2008).

[2]. Y. Zhao and D. G. Truhlar, Chem. Phys. Lett. 502, 1-13 (2011).