Supplementary data for article:

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Supporting Information

Stacking of Metal Chelates with Benzene: Can Dispersion-Corrected DFT Be Used to Calculate Organic–Inorganic Stacking?

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cphc_201402589_sm_miscellaneous_information.pdf

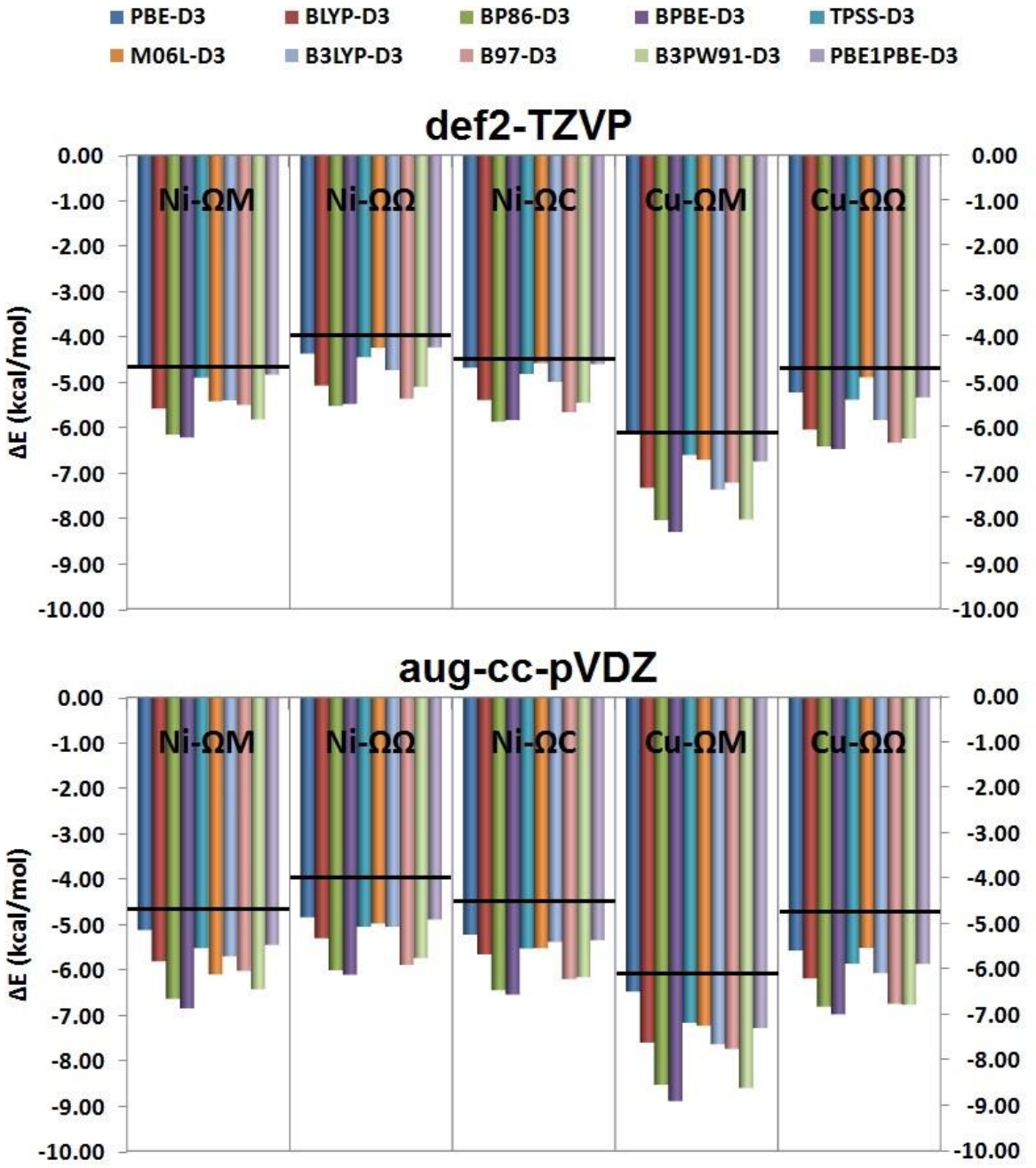

Figure S1. Performance of dispersion corrected GGA, H-GGA and M-GGA functionals for stacking interactions of metal-chelates with benzene, with def2-TZVP and aug-cc-pVDZ basis sets, and without BSSE correction; black lines within every system denote the benchmark CCSD(T) energy

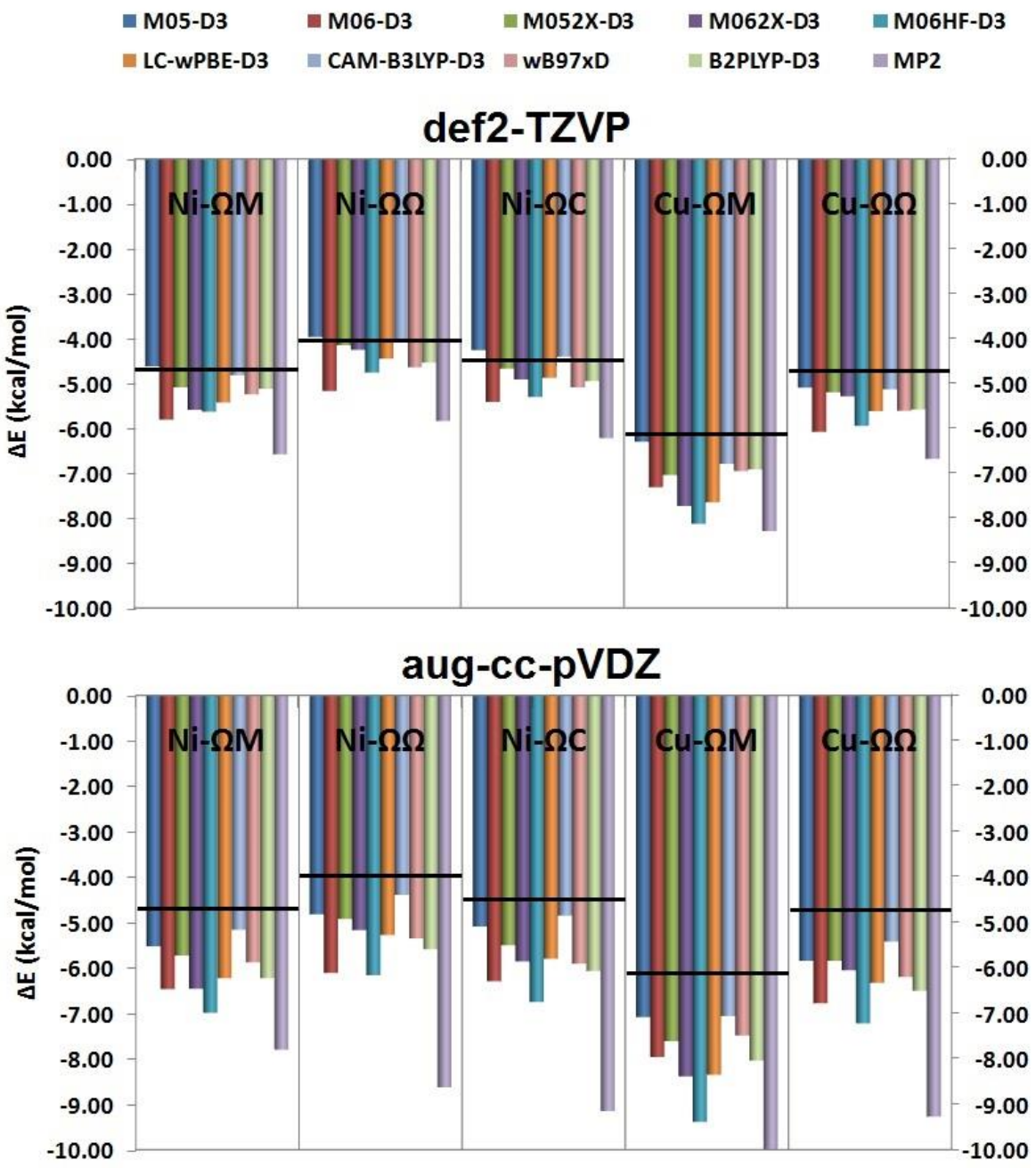

Figure S2. Performance of dispersion corrected HM-GGA, LC-GGA and DH-GGA functionals and MP2 method for stacking interactions of metal-chelates with benzene, with def2-TZVP and aug-cc-pVDZ basis sets, and without BSSE correction; black lines within every system denote the benchmark CCSD(T) energy