Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electron configuration and correlation effects in organometallic molecules from constraint density functional theory KENJI NAWA, KOHJI NAKAMURA, TORU AKIYAMA, TOMONORI ITO, Mie University, MICHAEL WEINERT, University of Wisconsin-Milwaukee — Interest in single organometallic molecule and that adsorbed on solid surfaces has rapidly increased because of possible novel applications. For molecules with transition metals (TMs), the *d*-electron configuration is an essential aspect of their electronic and magnetic properties, and correlation effects can not be excluded. Here, we investigate systematically the electron configuration and correlation effects for prototypical organometallic molecules of tridimensional metallocene ($TMCp_2$) and planer phthalocyanine (TMPc). Calculations were carried out based on the constraint density functional theory (DFT) by using the full-potential linearized augmented plane wave method that incorporates an on-site Coulomb interaction correction $+U$. We find that these correlation effects play a key role in determining the ground state of the electron configuration for the organometallic molecules. The calculated ground states of $TMCp_2$, where TM=Cr, Mn, Fe, Co, and Ni, obtained by constraint DFT with +U reproduce the experimentally determined structures of ${}^3E_{2g}$, ${}^6A_{1g}$, ${}^1A_{1g}$, ${}^2E_{1g}$, and ${}^3A_{2g}$, respectively. Results for the TMPc will be also presented.

Kenji Nawa
Mie University

Date submitted: 13 Nov 2014 Electronic form version 1.4