Supporting Information

Multivariate Linear Regression Models to Predict Monomer Poisoning Effect in Ethylene/Polar Monomer Copolymerization Catalyzed by Late Transition Metals

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Taking diimide palladium as an example, the single-point calculations were further performed at the higher level by using the density functional method M06, and 6-311+G (d, p) was used for the nonmetal atoms and the basis set LANL2DZ as well as the associated pseudopotential were applied for the Pd atom. In these single-point calculations, the solvation effect of toluene (ε = 2.37) was considered through the CPCM model.

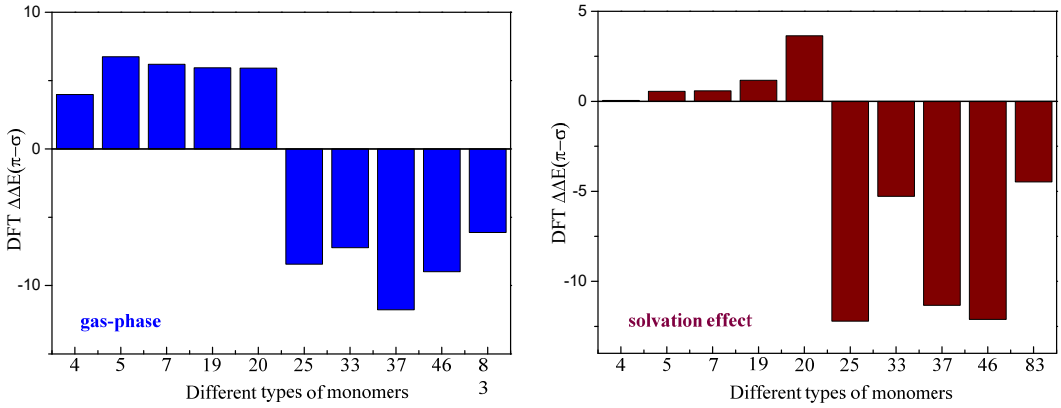

Figure S1. Gas-phase *vs*. solvation effect ΔΔ*E*(π-σ) (kcal/mol) for complex $\mathbf{II_{Pd}}$.

87 polar monomers

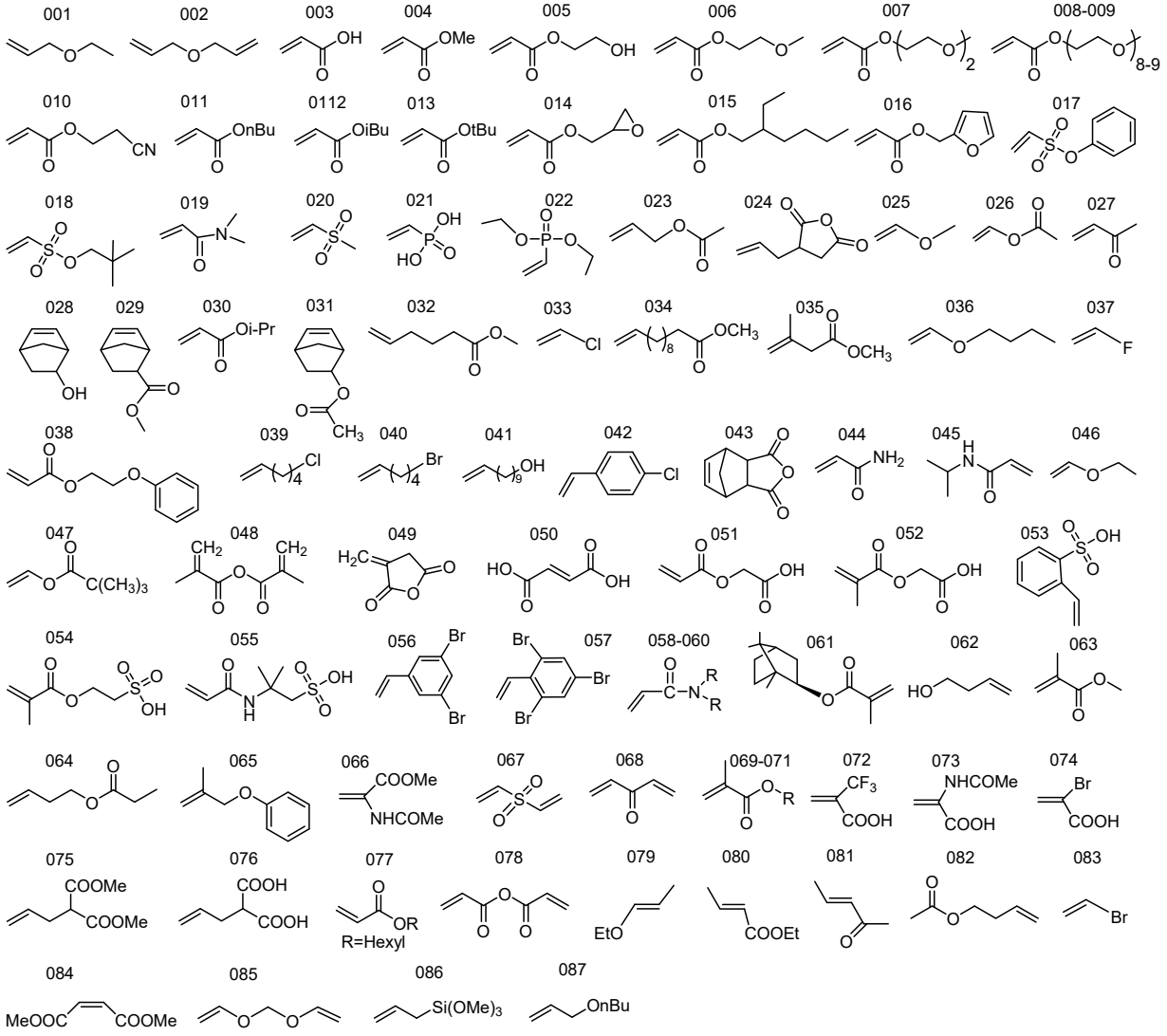

Figure S2. 87 polar monomers are used in the calculation of this work.

The descriptors of π-coordination structure **B3** (by complex $\mathbf{II_{Ni}}$) and polar monomers are calculated for multivariate linear regression. A total of 19 descriptors were calculated, including Sterimol values [50] ($^{B2}B1_{Ni\text{-}X}$, $^{B2}B5_{Ni\text{-}X}$ and $^{B2}L_{Ni\text{-}X}$), steric hindrance of metal center ($^{B3}Steric_{Ni}$), bond length ($^{B3}bond_{Ni\text{-}\pi\text{-}max}$ and $^{B3}bond_{Ni\text{-}\pi\text{-}min}$), Infrared freq ($^{mon}IR_{C=C}$) and Freq Intensities ($^{mon}\nu_{C=C}$), NMR ($^{mon}NMR_C^{\alpha}$, $^{mon}NMR_C^{\beta}$ and $^{mon}NMR_X$), NBO ($^{B3}NBO_{Ni}$, $^{mon}NBO_X$, $^{mon}NBO_C^{\alpha}$ and $^{mon}NBO_C^{\beta}$), Polarizability ($^{mon}\alpha$), HOMO (^{mon}HOMO), volume (^{mon}V) and Dipole Moment ($^{mon}\mu$).

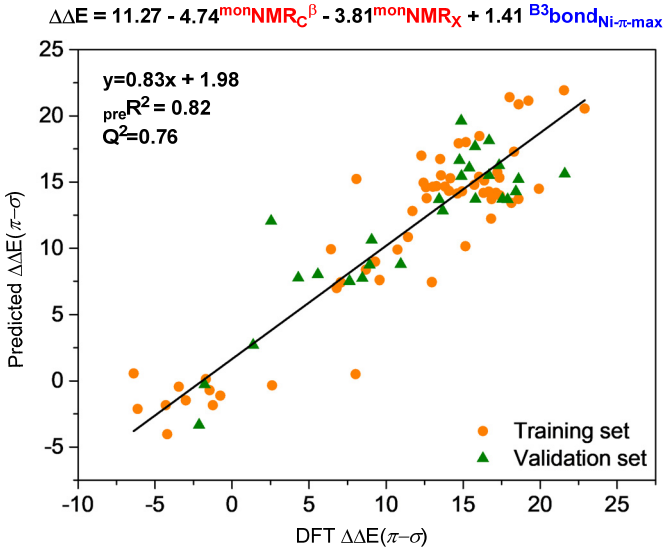

Figure S3. Plot of computed *vs*. predicted ΔΔ*E*(π-σ) (kcal/mol) for complex $\mathbf{II_{Ni}}$ (base on π-coordination structure) using the multivariate linear regression models.

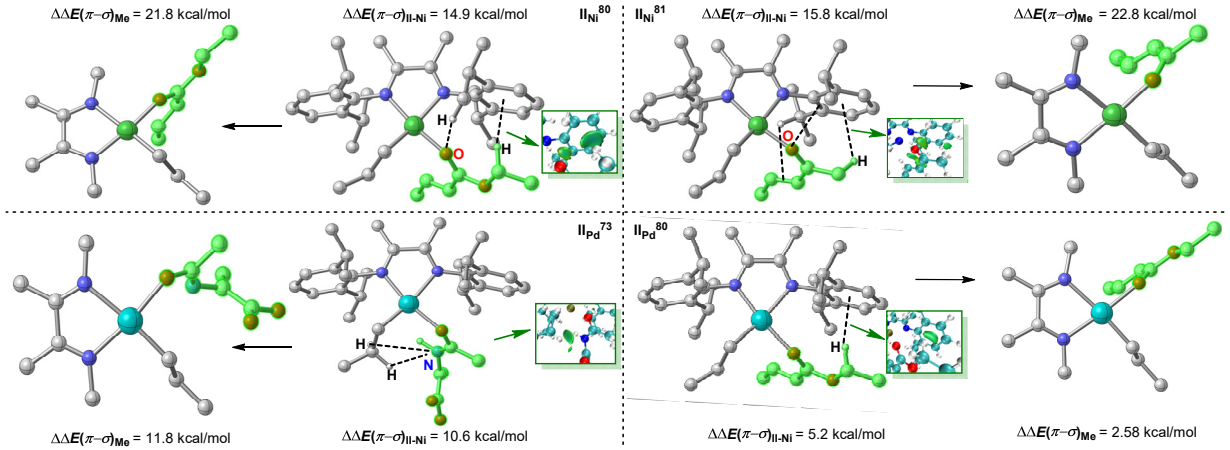

Figure S4. Changes of structure and ΔΔ*E*(π-σ) after substitution of aromatic ring on catalyst (complex $\mathbf{II_{Ni}}$) with methyl.