[P1] Development of Organometallic Force Field for Soft Crystal

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"Soft crystal" is one of new materials that a "hard" crystal structure easily changes to another one by specific low energy stimulation at room temperature, and is expected the creation of innovative material functions by controlling its metastable states and their crystal polymorphic transitions. In this study connected to the brand-new research project, to build the theory for the formation mechanism and the transition phenomenon of the novel "soft crystals", our research group develops the innovation technologies [1,2]; (1) Construction of a crystal force field potential capable of precisely and promptly evaluating the molecular crystal structure formed by organometallic complexes. (2) Development of an efficient crystal polymorphism search method that can find many meta-stable polymorphic states which is not observed experimentally but is plausible existence. (3) Computational chemistry approaches for giving theoretical investigations of crystal phase transition phenomenon of "softcrystal" based on the meta-stable polymorphic states found and their transition dynamics simulation.

Our first targets including metal complexes are (a) aryl-isocyanide gold compounds [3] and (b) lanthanoide complexes with bisbipyridinly ethylenediamine derivatives [4] as shown in Figure 1.

In this work, we determined the organometallic force field parameters of their metals, Au and lanthanoides; Nd, Eu, Gd, Tb, and Ho, to reproduce the soft crystal structures of their complexes. Geometry optimizations of their molecular crystal structures are carried out by CONFLEX software [1].

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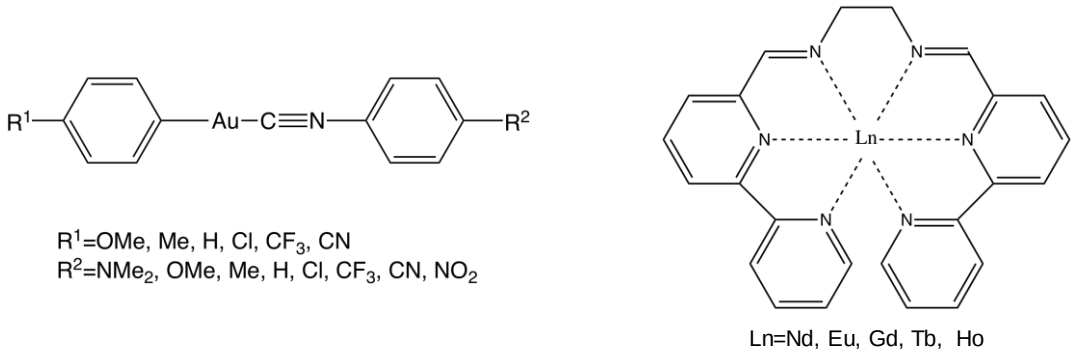

(a) (b)

Figure 1 Target Organometallic Compounds

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