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A reparametrization approach of the B3LYP functional based on the equilibrium temperature of the spin crossover AHMED SLIMANI, XUEFANG YU, Department of Chemical System Engineering, The University of Tokyo 7-3-1, Hongo, Bunkyo-Ku, Tokyo 113-8656, Japan, AZUSA MURAOKA, Department of Physics, Meiji University 1-1-1, Higashi-Mita, Tama-Ku, Kawasaki-shi, Kanagawa 214-8571, Japan, KAMEL BOUKHEDDADEN, Groupe d'Etude de la matière Condensée, CNRS-Université de Versailles 45, Avenue des Etats Unis, 78035 Versailles, France, KOICHI YAMASHITA, Department of Chemical System Engineering, The University of Tokyo 7-3-1, Hongo, Bunkyo-Ku, Tokyo 113-8656, Japan — The theoretical study of the electronic structure of spin crossover compounds is very challenging due to the technical limitations of highly accurate ab-initio methods and/or the inaccuracies of density functional methods in the prediction of low-spin/high-spin energy splitting. However, calculations using the reparametrized functionals could improve the results. We present an investigation of the HS/LS energy gap of a typical spin crossover compound using several DFT functionals. We propose a reparametrization approach based on the equilibrium temperature of the spin crossover compounds leading to reasonable estimation of the HS/LS energy gap. In fact, the proposed approach is very important to match the used functional to the considered spin crossover compound.

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