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Spin-Charge Coupling and Charge Order Phases in $LuFe_2O_4$ CHANG-JONG KANG, B.I. MIN, POSTECH — Possible charge order phases in mixed-valent multiferroic $LuFe_2O_4$ are studied based on the first principles density functional theory. We have considered two different charge order phases of $LuFe_2O_4$ suggested by Angst et al. [1] and de Groot et al. [2], and investigated their electronic and magnetic properties systematically to determine the correct charge order phase that is consistent with the experiment. The systematic comparison of physical properties between two charge order phases will be discussed, and the corresponding spin-charge coupling effect will be examined. We have found that the spin-charge coupling effect is an essential ingredient in $LuFe_2O_4$.

[1] M. Angst et al., Phys. Rev. Lett. 101, 227601 (2008).

[2] de Groot et al., Phys. Rev. Lett. 108, 187601 (2012).

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