Strain Effect on the Magnetic Properties of Pd: the First Principles Study

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In this study, different correlation functions have been applied to investigate magnetic properties of palladium (Pd). While GGA show the magnetic moment of Pd up to 1.1 \( \mu_B \), no magnetic moment was found when LDA is used. To understand the difference between magnetisms in LDA and GGA, the detail electronic structures of Pd using LDA and GGA are compared to each other and discussed in detail. The strain effects on electronic and magnetic properties of both bulk and thin film of Pd are also calculated and discussed.

*This work is supported by grants from the Priority Research Centers Program (Grant No. NRF-2009-0093818) and the Basic Science Research Program (Grant No. NRF-2015R1A2A2A01003621) through NRF funded by the MOE and MSIP of Korea.