Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Density-matrix renormalization group studies on a magnetic impurity in graphene TOMONORI SHIRAKAWA, RIKEN, RIKEN AICS, CREST, SEIJI YUNOKI, RIKEN, RIKEN AICS, CREST, RIKEN CEMS — Motivated by recent experiments on the emergence of magnetism in graphene induced by lattice defects or by magnetic adatoms, we have theoretically studied the ground state properties of single magnetic impurity in grapheme. First, we have developed a new numerical technique within the density-matrix renormalization group (DMRG) scheme for magnetic impurity model in general to study site-dependent quantities including local density of states even away from magnetic impurity site, Friedel density oscillations, and spin-spin correlation functions between the magnetic impurity and the surrounding conduction electrons. This new technique is applied to three different models: (i) a magnetic adatom on grapheme, (ii) a substitutional magnetic impurity in grapheme, and (iii) a model on defect in the graphene. Our systematic study of these models reveals that, in the presence of particle-hole symmetry, the ground state of model (i) exhibits the formation of local moments without Kondo-screening, whereas the others behave very similarly to the Kondo singlet states. We also discuss the real-space decay of spin-spin correlations between magnetic impurity and surrounding conduction electrons in these models.

Tomonori Shirakawa
RIKEN

Date submitted: 15 Nov 2013 Electronic form version 1.4