Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Influence of spin-orbit coupling on the multiorbital Hubbard model: J-freezing, Hund's rules and excitonic magnetism AARAM J. KIM, HARALD O. JESCHKE, Goethe University Frankfurt am Main, Germany, PHILIPP WERNER, University of Fribourg, Switzerland, ROSER VALENTI, Goethe University Frankfurt am Main, Germany — We investigate the interplay between the spin-orbit coupling, Coulomb interaction and Hunds coupling within the multiorbital Hubbard model at different fillings by means of the dynamical mean-field theory combined with continuous-time quantum Monte Carlo. We show that the spin-freezing crossover occurring in the metallic phase of the model without the spin-orbit coupling can be the generalized to a **J**-freezing crossover with $\mathbf{J} = \mathbf{L} + \mathbf{S}$, in the spin-orbit-coupled case. In the **J**-frozen regime the correlated electrons exhibit a non-trivial flavor dependence in the self-energy which cannot be captured by the effective crystal-field effect. Especially, in the regions near $n = 2$ and $n = 4$ the metallic phases show strong asymmetry from each other, which reflects the atomic Hunds third rule. Finally, we explore the appearance of the excitonic magnetism near $n = 4$ and discuss the relevance of our results for real materials.[1]

[1]A. J. Kim *et al.*, arXiv:1607.05196.

Aaram J. Kim
Goethe University Frankfurt am Main, Germany

Date submitted: 10 Nov 2016 Electronic form version 1.4