



Localization in Energy Materials

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Thursday

November 16

4:00 P.M.

Rm 184 NSH

Disorder is ubiquitous in materials and can drastically affect their properties. In particular it can induce localization of electrons and lead to a metal-insulator transition, which is known as the Anderson localization transition. Anderson localization is not only interesting from a scientific point of view, but also has been proposed to play a critical role in materials that can be used for the harvesting and efficient use of energy. Combining two recently developed methods, the effective disorder Hamiltonian method[1] and the typical medium dynamical cluster approximation[2], has opened the door to investigate localization in such energy materials with first principles simulations. In this talk, I will present our recent studies of localization in the Fe based superconductor $KxFe_2-ySe_2$ [3], the diluted magnetic semiconductor $Ga(Mn,N)$ [4] and the intermediated-band photovoltaic Ti doped Si.

[1] T. Berlijn, D. Volja, and W. Ku PRL 106, 077005 (2011)

[2] C. E. Ekuma, H. Terletska, K.-M. Tam, Z.-Y. Meng, J. Moreno, and M. Jarrell, PRB 89, 081107 (2014)

[3] Y. Zhang, H. Terletska, C. Moore, C. Ekuma, K.-M. Tam, T. Berlijn, W. Ku, J. Moreno, and M. Jarrell, PRB 92, 205111 (2015)

[4] Y. Zhang, R. Nelson, E. Siddiqui, K-M Tam, U. Yu, T. Berlijn, W. Ku, NS Vidhyadhiraja, J. Moreno, and M Jarrell, PRB 94, 224208 (2016)